

### **Method for analysing metabolites**

The present application relates to a method for analysing the metabolites of a biological sample which comprises quantitatively determining one or more metabolites in said sample in a way that said quantitative determination resolves isotopic mass differences within one metabolite, said method being characterized in that the sample comprises or is derived from a cell which has been maintained under conditions allowing the uptake of an isotopically labeled metabolizable compound so that the metabolites in said cell are saturated with the isotope label. This method may further comprise, prior to quantitatively determining the metabolites, combining the biological sample (i.e. the first biological sample) with a second biological sample in which the metabolites are not isotopically labeled or are isotopically labeled differently from the first biological sample; and determining in said biological samples the relative quantity of metabolites which differ by their isotopical label. The present invention also relates to sets of isotopically labeled metabolites obtainable by applying this method, as well as to kits facilitating the application of this method and to corresponding uses.

The present invention belongs to the field of metabolome analyses, also referred to as metabolic profiling, i.e. the quantitative analyses of metabolites in a biological sample with the aim to investigate the state of organisms in particular with respect to biochemical regulatory networks. In the prior art, the metabolome, besides the proteome, transcriptome and genome, has become the fourth cornerstone of biological systems analyses. Only metabolome analyses allows insight into nutrient use, biosynthetic capacity of organisms, signalling and communication mediated via low molecular weight compounds and biochemical adaptive processes. Therefore profiling analyses of relative changes of all metabolites within an organism is in demand for a true biological systems analysis.

Metabolome analyses are still in early development inter alia because, in contrast to genome, transcriptome and proteome analyses, metabolome analyses has to deal with a highly diverse range of chemicals covering substances from small molecular

weight volatiles up to polymers. Conventionally, different and specialised analytical platforms are used in order to analyse these different classes of compounds. Meanwhile, universally applicable analytical platforms have been developed for complex mixtures of compounds. These exploit molecular mass and chromatographic retention in so-called hyphenated technologies, like GC-MS, HPLC-MS or MALDI-TOF. Bench-top gas chromatography coupled to mass spectrometry (GC-MS) was the first technology platform proposed for large-scale metabolome analyses (Trethewey, 1999). The choice of this hyphenated technology took into regard the ideal combination of unsurpassed chromatographic separation with high selectivity, sensitivity, and dynamic range of quantitative mass detection. Moreover, both GC and electron impact ionisation (EI) mass spectrometry exhibit only minor matrix effects as compared to other MS techniques, as for example matrix assisted laser desorption/ionisation-time of flight (MALDI-TOF) (Guo, 2002) mass spectrometry or liquid chromatography coupled to mass detection (HPLC-MS) (Matuszewski, 2003). High reproducibility of the GC-MS analyses of metabolites, which routinely uses methoxyamine hydrochloride (MEOX) and N-methyl-N-(trimethylsilyl)-trifluoroacetamide (MSTFA) reagents, allowed metabolite profiling based on external quantification of respective methoxyamine (MX) and trimethylsilyl (TMS) derivatives (Fiehn, 2000a; Roessner, 2000; Roessner, 2001). The scope of metabolites covered is, however, limited (1) by the required volatility of metabolites or stable chemical derivatives of unstable metabolites, and (2) by the distribution of metabolite concentrations within each type of sample. The maximum sample load of any multi-parallel chemical analyses is determined by the predominating metabolites. GC-MS metabolite profiles have an enormous dynamic range of 4 to 5 orders of magnitude. The upper limit of quantification is set by the requirement for surplus chemical reagent and by peak deformation effects due to chromatographic overloading. Thus, biological matrices devoid of single predominant metabolites promise best potential for highly complex multi-parallel analyses (Fiehn, 2000a; Roessner, 2000).

Two main strategies are conceivable toward a more comprehensive metabolome analyses: (1) the choice of other analytical techniques which may supplement GC-MS analyses, and (2) the application of pre-fractionation and concentration techniques for the enrichment of trace compounds. However, both strategies are currently highly limited. Supplementary MS techniques, as for example MALDI-TOF-



MS or HPLC-MS, are subject to strong interferences, which result from the changing compositions of complex biological matrices. These so-called matrix effects may lead even to complete suppression of ionisation and response signal (Matuszewski, 2003; Guo, 2002). On the other hand, most pre-fractionation and concentration techniques result in high or highly variable losses of metabolites.

These drawbacks preventing the use of potentially more powerful MS techniques in metabolite profiling studies may at least in part be overcome by including internal standards into the metabolite analyses. Indeed, a thorough quantitative standardisation for as many as possible measured metabolites is required. This would make it possible to extend the scope of metabolite profiling to such techniques, because it would allow an exact quantification of the metabolite levels for which a standard is available. From investigations on metabolic fluxes, it is known that metabolites can be labeled in vivo with a stable isotope (Wittmann, 2002). However, flux analyses are generally confined to the investigation of very limited biochemical pathways and do not cover metabolites in the breadth as is normally required for metabolic profiling. Consequently, the substrate compounds which are used in such studies in order to label cells with a stable isotope are typically very specific to the particular biochemical pathway to be analysed. Their production is expensive because it requires specific and time-consuming chemical syntheses.

To summarize, a practicable approach for establishing a quantitative standard for use in metabolite profiling is not in sight in the prior art. This is mainly explained by the diversity of compound classes to which metabolites may belong and by the fact that most of the metabolites cannot be tagged after extraction as it is possible for the chemically uniform transcripts and proteins (see, e.g., Gygi, 1999).

Thus, the technical problem underlying the present invention is the provision of means and methods that allow it to improve metabolome analyses by establishing a reliable quantitative standard for as many as possible metabolites in order to broaden the scope of such analyses.

This technical problem is solved by the provision of the embodiments as characterized in the claims.

Accordingly, the present invention relates to a method for analysing the metabolites of a biological sample which comprises quantitatively determining one or more metabolites in said sample in a way that said quantitative determination resolves isotopic mass differences within one metabolite, said method being characterized in that the sample comprises or is derived from a cell which has been maintained under conditions allowing the uptake of an isotopically labeled metabolizable compound so that the metabolites in said cell are saturated with the isotope with which said metabolizable compound is labeled.

The present invention is based on the experiments described in the appended Examples which show that it is possible to label substantially all possible metabolites in vivo. The proof that this principle works has been obtained by labeling yeast cells with U-<sup>13</sup>C-glucose. This work represents the keystone to comprehensive, fully quantitative metabolome profiling and will greatly facilitate future developments within this field. It solved the technical problem of standardisation by differential labeling of metabolites with isotopes. Similar to differential labeling of transcript samples by fluorescent probes or of protein samples by chemical tagging, it is possible in the method of the present invention to tag the metabolome by saturating in-vivo labeling with isotopes. This concept can be extensively exploited for a non-biased sampling of mass spectral metabolite tags (MSTs) and isotopomer ratio (ITR) metabolite profiling. In particular, isotope-saturated extracts produced by the method of the invention may be used as a multiplex mixture of internal standards, where each component of the resulting metabolite profiles will be quantified relative to the respective fully labeled isotopomer (see Example 4 and Figure 2). It is envisaged that these achievements, in particular the compilation of a first compendium of MSTs which, analogous to ESTs, allows qualitative assessment of the metabolome composition and the demonstration of fully quantitative ITR metabolite profiling, will greatly improve metabolome analyses.

In the prior art, isotope labeling studies are routine approaches used for metabolite flux analyses (Wittmann, 2002; Christensen (1999); Wiechert, 2001. These studies require isotopically labeled compounds, which are expensive and of limited availability. In a conventional flux experiment, a labeled compound is fed to

organisms, which are pre-grown on media with ambient isotope distribution (dos Santos, 2003; Lee, 1991) resulting in the labeling of a corresponding specific isotopically labeled metabolizable compound. However, flux studies differ from the method of the invention in that they generally involve partial labeling of the metabolites of a cell. This is explained by the fact that flux studies require partial, i.e. incomplete, labeling. By contrast, the method of the present invention achieves saturating labeling which means a labeling of the metabolites as complete as possible given the degree of labeling in the isotopically labeled metabolizable compound used to label the cell from which the biological sample for analyses is derived (for more detailed definitions see below).

One advantage of the present method is the fact that it introduces an isotopic label at the site which is ideal for metabolome analyses, namely the active biological sample. In prior art technologies, a differential label is often introduced only in the course of chemical analyses such as in the currently prevailing methods for quantitative proteome (Aebersold, 2003) and transcriptome (Duggan, 1999) analyses. These technologies for example involve isotope-coded protein-tagging techniques (Gygi, 1999) and two-colour labeling by fluorescent probes (Schena, 1995; Lockhart, 1996). However, labeling only after extracting the respective compounds from the cell may introduce a bias in the labeling result. Such artefacts are excluded in the method of the invention.

Apart from incorporation of label in the course of chemical analyses, there has been at least one approach to label proteins in vivo. Oda (Proc. Natl. Acad. Sci. USA 96 (1999), 6591-6596) describe whole cell-labeling for proteome analyses using the stable isotope  $^{15}\text{N}$ . However, in vivo isotope labeling of the entire set of metabolites has not been reported in the prior art. In particular, by using  $^{13}\text{C}$ -labeling of yeast cultures, the present invention demonstrates that combined mass spectral analyses of differentially labeled samples, especially  $^{13}\text{C}$ -ITR profiles, can be generated. In particular, the experiments underlying the present invention surprisingly show that complete (i.e. saturating) labeling of metabolites could be achieved in yeast cells. The results obtained in the appended Examples are surprising because it could not have been excluded that carbon sources other than the isotopically labeled metabolizable compound (in the examples  $\text{U-}^{13}\text{C}$ -glucose) which are present in the medium could have prevented an efficient broad isotope labeling of the metabolites.

## 6.

It is almost impossible to avoid in the medium the presence of such other carbon sources like for instance essential nutrients, such as vitamins, or auxotrophic markers. The processing of these compounds in the cultured cells could have severely interfered with isotope labeling and thereby prevented the required saturating labeling. However, as is shown in the Example experiments, the lack of labeling in the cell due to the presence of the unlabeled carbon sources in the medium is greatly restricted to the compounds themselves or to direct metabolic products thereof (see Example 1). A mixing of label with unlabeled compounds essentially did not take place. This was surprising and means that in vivo labeling with isotopes can indeed be applied for achieving broad coverage of the metabolites with isotopic labeling.

Another surprising finding was that the presence of isotope label in the metabolites does not substantially influence the distribution of metabolite levels in the sample when it is compared with a metabolite profile obtained from a corresponding unlabeled sample (i.e. a sample, wherein the cells have been fed with nutrients in which the isotopes are present in the naturally occurring, i.e. ambient proportions). This is for example evident from the results depicted in Figure 2 and described in Example 4. This could not have been expected since it is known that enzymes may discriminate between isotopomers. For instance, such effects are described from plant physiology such as for RUBISCO, CO<sub>2</sub>-fixation and phosphoenolpyruvate carboxylase (PEPC) (see, e.g., Le Roux-Swarthout, J. Plant Physiol. 157 (2000), 489-493) and from fungi, yeast or other microorganisms, e.g., for pyruvate decarboxylase (PDC), and the isoprenoid metabolism (see, e.g., Stivers, Biochem. 32 (1993), 13472-13482; Henn, Appl. Environ. Microbiol. 66 (2000) 4180-4186; Londry, Appl. Environ. Microbiol. 69 (2003), 2942-2949). Thus, it was reasonable to expect that, caused by isotope discrimination, the labeling of metabolites with isotopes would influence the distribution of metabolite levels in the biological sample. But, as it is shown herein, the isotopically labeled metabolites show a distribution that greatly corresponds to that obtained for unlabeled metabolites. This proves suitability of the method of the invention for standardizing metabolite analyses.

The experimental results summarized in the following show that the method of the invention may become an indispensable tool for the future development of metabolite profiling.

The present invention is herein exemplified in experiments using a *Saccharomyces cerevisiae* model which was subjected to saturating in vivo stable isotope labeling by growing on an exclusive  $^{13}\text{C}$ -source (see, e.g., Figures 1 and 9). The in vivo labeling of metabolites in yeast generates isotopomer tags which could be differentially detected by mass spectrometry. When applied as internal quantitative standard, isotope-labeled compounds may facilitate a meaningful quantitative analyses if for example two samples, the one being saturatingly labeled and the other not being labeled (i.e. having ambient isotope abundances) are compared and the relative ratio between each isotopomer tag and the corresponding unlabeled metabolite is determined. Interestingly, this working principle may even facilitate those mass spectral technologies such as MALDI-TOF-MS which are prone to matrix suppression effects and high variability and which therefore hitherto were not applied for quantitative metabolite profiling analyses. An example of successfully using the method of the invention by applying MALDI-TOF-MS is presented herein (Example 9 and Figure 9). This means that the method described herein may allow to extend multi-parallel metabolite profiling in principle at least to all mass spectrometry-based technologies.

A further advantage of the method of the invention over conventional metabolome analyses is that it allows an immediate proof of the metabolic origin of any mass spectral tag which is detected in biological samples. While protein and mRNA sequence diversity provides information about the source species by the sequence information contained therein, the origin is not immanent in metabolite structure per se, except for the subset of species-specific secondary metabolites. However, as soon as a pair of labeled and non-labeled MSTs is found, chemical artefacts or laboratory contaminations can immediately be ruled out.

In addition, mass shifts allow a direct insight into the number of carbon atoms present within each compound or fragment. This property of the method of the invention increases the insight into the chemistry of those MSTs the chemical nature of which is unknown and may support the identification of MSTs by other techniques (Table 3).

In analogy to expressed sequence tags (ESTs), identified and non-identified MSTs may be used as a highly useful tool to characterise the metabolome of any biological sample. Again in analogy to tools for sequence comparison, MSTs can easily be

identified by matching of mass spectral fragmentation and chromatographic retention. Furthermore, clustering technologies allow a meaningful classification of MSTs (Figure 4) (Wagner, 2003).

As a further advantageous property, the method of the invention allows a fast investigation of the precision of analytical methods which are being developed for metabolite profiling. In addition, it makes quantitatively standardized metabolome analyses accessible to biological samples which are obtained by pre-purification and enrichment of fractions of the total metabolite extract taken from a biological sample, for instance in order to detect trace metabolites. In the prior art, such samples fall below the detection limits of conventional GC-MS profiling. The possibility of the method of the invention to quantitatively determine minor amounts of metabolites facilitates to conduct metabolite co-response analyses which may provide direct information about quantitative metabolite interactions in biological systems. Such interactions may be expected based on theoretical considerations (Steuer, 2003). Observed metabolite co-responses may be uncoupled or may follow linear functions. Metabolite co-response may be either constitutive or conditional with respect to the set of experiments under investigation. In Example 8, metabolite co-response analyses applying the method of the invention are described. Accordingly, metabolite co-responses may best be discovered and judged by a set of different distance measures, among which the Euclidian distance is least indicative (Figure 6). Metabolite interactions may reflect canonical pathway definitions (Figure 7), but may also allow to discover cross-pathway interactions (Figure 8). Investigations into these interactions are highly valuable, because they can provide insights into common mechanisms of metabolic control. However, to date, such analyses are restricted due to the limited coverage of metabolome data. Based on the extension of metabolite data mining that is now possible by applying the method of the invention, for instance because of the possibility to exploit MALDI-TOF for quantitative determination of metabolite levels on a broad scale, it is conceivable that the present invention will further the development of quantitative metabolome analyses, in particular towards trace compounds and general co-factors.

As it is explained above, the present invention belongs to the field of the metabolic profiling or metabolome analyses. This means that the method of the invention is of use for quantitatively determining one or more metabolites in a biological sample.

The term "quantitative determining" refers to the determination of the relative or absolute amount of each analyzed metabolite in the sample. Generally, such a determination leads to a so-called metabolite profile pertaining to the respective biological sample. Such metabolite profiling approaches have been carried out in many laboratories and therefore belong to the prior art.

Since isotopic labeling is applied in the method of the invention, it is necessary that the technique used to quantitatively determine the metabolites resolves isotopic mass differences as they may occur within one metabolite. Compounds that differ from one another only by one or more isotopes incorporated into the chemical structure are generally referred to as "isotopomers". The technique used to detect the metabolites must therefore be capable of discriminating between two compounds that differ in their mass by as little as one relative atomic mass. Corresponding techniques are known to the skilled practitioner and described in the literature. They involve different kinds of mass spectrometry or NMR, as is described in further detail further below.

The term "isotopic labeling" is to be understood to refer to compounds that are labeled with an isotope that is not the main isotope of the element of said isotope. "Labeled" means in this context to have a significantly and, for detection purposes, usefully increased proportion of the label-isotope as compared to the abundance of said isotope occurring in nature, preferably the proportion of the label-isotope is increased to at least 80%, more preferably to at least 90% and even more preferably to at least 95% and most preferred to at least 99% of the total of all isotopes of the respective element. The term "isotopic labeling" furthermore preferentially refers to compounds in which the label-isotope is present in the above-mentioned proportion at each possible position within the chemical structure of the compound. However, partial labeling of compounds may also be of use in the context of the present invention. Such applications require that means of correction for the proportion of residual non-labeled isotopomers are applied. In this case, labeling needs to be saturating, i.e. the proportions of isotopomers for each metabolite needs to be constant in the labeled sample, so that the isotopomer proportions can be

determined in a control experiment and used for mathematical correction of the metabolite profiling results. Preferably, the isotopically labeled metabolizable compound used in order to label the cell contains of the respective element only the label-isotope (in the proportion that is technically feasible) as it is the case with U- $^{13}\text{C}$ -glucose where all six carbon atoms are the  $^{13}\text{C}$  isotope.

The method of the present invention is characterized in that the sample comprises or is derived from a cell which has been maintained under conditions allowing the uptake of an isotopically labeled metabolizable compound so that the metabolites in said cell are saturated with the isotope with which said metabolizable compound is labeled.

It is a critical feature of the method of the invention that the metabolites are saturated with the isotopic labeling. "Saturated" (or "saturating labeling") means that the metabolites in the cell or the biological sample derived therefrom contain an amount of isotope label that substantially corresponds to the amount of label in the metabolizable compound taken up by the cell in order to label it, and that substantially all of the metabolites to be analyzed contain the isotope label. In particular, "saturating labeling" refers to an amount of labeling of the metabolites to be analyzed so that these metabolites overall contain at least 50%, preferably at least 70%, more preferably at least 80%, still more preferably at least 90% and most preferably at least 95% of the amount of isotopic label as present in the isotopically labeled metabolizable compound. The term "substantially all of the metabolites to be analyzed contain the isotope label" means that at least 70%, preferably at least 80%, more preferably at least 90%, still more preferably at least 95% and most preferably at least 98% of the metabolites to be analyzed are labeled, i.e. differ by at least one relative atomic mass from the corresponding unlabeled counterpart. Preferably, substantially all of the metabolites to be analyzed contain the isotope label if at least 20, more preferably at least 50, still more preferably at least 100, even more preferably at least 150 and most preferably at least 200 or even at least 300 metabolites of the biological sample to be analyzed contain the isotopic label.

Exceptions to the labeling to saturation may be tolerated, however, should be taken into account when analysing the metabolite data obtained. Non-labeled metabolites may be present in the biological sample when, in addition to the isotopically labeled metabolizable compound, other compounds, for example essential nutrients like



metabolizable compound, other compounds, for example essential nutrients like vitamins or auxotrophy markers, have been provided to the cell via the culture medium and these compounds do not contain the isotope label. Therefore, it may happen that cells which are labeled to saturation contain unlabeled metabolites which are these other compounds or metabolic products thereof.

The number and selection of metabolites analyzed in the method of the invention depends on the goal to be achieved by carrying out the method of the invention. It is typical for metabolic profiling like the method of the invention to aim at quantitatively determining an as large as possible subset of metabolites in order to obtain as much as possible metabolite data. Here, the possibility to label in principle each metabolite by the method of the invention is a big advantage over prior art approaches because it provides a quantitative standard for each metabolite to be analyzed.

Accordingly, in a preferred embodiment of the method of the invention, at least 20, more preferably at least 50, still more preferably at least 100, even more preferably at least 150 and most preferably at least 200 or even at least 300 metabolites are quantitatively determined.

The term "metabolite" refers to any substance within a cell or produced by a cell, including secreted substances, which can be quantitatively determined by applying the method of the invention, that is for which suitable techniques for determining the amount are available. Preferably, these substances are not macromolecules (i.e. biopolymers) such as DNA, RNA or proteins. Particularly preferred are metabolites with a low molecular weight preferably the metabolites have a molecular weight of not more than 4000 Da, preferably not more than 2000 Da, more preferably not more than 1000 Da. Typically, the metabolites to be analyzed may belong to the following, non-limiting list of compounds: carbohydrates (e.g. sugars, oligo- and polysaccharides such as polyglucans as for example starch or polyfructans), sugar alcohols, amines, polyamines, amino alcohols, aliphatics, aliphatic alcohols, amino acids, lipids, fatty acids, fatty alcohols, organic acids, organic phosphates, organic ions, other inorganic ions bound to metabolites, nucleosides, nucleotides, sugar nucleotides, purines, pyrimidines, such as adenine and uracil, sterols, terpenes, terpenoids, flavons and flavonoids, glucosides, carotenes, carotenoids, cofactors,

ascorbate, tocopherol, vitamins, polyols, organic amines and amides such as ethanol amine and urea and/or heterocyclic compounds such as nicotinic acid.

As is evident from the appended Examples, the method of the invention also involves analysing metabolites of which the chemical nature is unknown. However, metabolites (herein also referred to as "mass spectral metabolite tags" or "MSTs") of unknown chemical nature may nevertheless provide informative data on the biological sample analysed. It is clear that, if a metabolite of unknown chemical nature is revealed by carrying out the method of the invention to have an interesting property or diagnostic value or characteristic behaviour, this metabolite may be further characterized by applying suitable analytical methods known in the art.

In a particularly preferred embodiment, the method of the invention refers to the quantitative determination of metabolites comprising sugars, sugar alcohols, organic acids, amino acids, fatty acids, vitamins, sterols, organic phosphates, polyamines, polyols, nucleosides, purines, pyrimidines, adenine, uracil, organic amines and amides such as ethanol amine and urea and/or heterocyclic compounds such as nicotinic acid.

The isotope used for in vivo labeling in connection with the present invention may be selected among available isotopes that may be suitable for applying the method of the invention. As a preferred selection, a skilled person may use an isotope for which corresponding isotopically labeled metabolizable compounds are available, in particular commercially available. As a further preferred choice, isotopes for use in the method of the invention should be such that they do not harm viability of the cells from which the biological sample for analyses is taken or that they do not interfere with the metabolism such as by influencing the activity of metabolic enzymes. In this regard, it is thus preferred to use stable isotopes rather than radioactive ones. As a further aspect, one should take into account that elements such as carbon or hydrogen are preferred over elements that are present in metabolites more rarely in order to cover the metabolites of a cell by in vivo labeling as completely as possible. Particularly preferred isotopes are  $^{13}\text{C}$ ,  $^{15}\text{N}$ ,  $^{18}\text{O}$  and  $^2\text{H}$ , with particular preference of  $^{13}\text{C}$ .

The label-isotope is incorporated into the cells from which the biological sample for analyses is taken by maintaining the cell under conditions allowing the uptake of said compound. This means that the compound should be one that is readily taken up by the cells and that is also readily metabolized so that it is ensured that saturation with the isotopic label can be achieved. Depending on the kind of cells or organism to be labeled, the label may for example be provided by feeding cultured cells such as yeast cells or mammalian cells with a nutrient, e.g. a carbon source if the label is  $^{13}\text{C}$ . If the cells to be labeled are within a multicellular organism, the label may be incorporated by subjecting the labeled metabolizable compound through the substrate (e.g. the water) if it is a plant or by injecting the labeled compound into it if the organism is an animal, for instance a vertebrate, in particular a mammal.

As the isotopically labeled metabolizable compound, substances should be used that provide for an effective uptake of the label by the cell. Preferably, the compound may be totally labeled with the isotope (i.e. no atom of the respective element in the compound is of another isotope than the label-isotope). Corresponding labeled compounds may be available from commercial suppliers such as those mentioned in the Examples. Particularly preferred isotopically labeled metabolizable compounds are  $\text{U-}^{13}\text{C}$ -glucose,  $^2\text{H}_2\text{O}$ ,  $\text{H}_2^{18}\text{O}$ ,  $\text{U-}^{13}\text{C}$  acidic acid,  $^{13}\text{C}$  carbonate and  $^{13}\text{C}$  carbonic acid.

The term "biological sample" encompasses any amount of material comprising cells or derived from a cell that is susceptible to the method of the invention. In the present context, the term "cell" refers to any conceivable living entity that is capable of being in vivo-labeled according to the teachings of the present invention. Accordingly, the method may be applied to any type of cell, prokaryotic or eukaryotic cells, viral particles, wild-type or transformed, transduced or fused cells, or derivatives thereof such as membrane preparations, liposomes and the like. The cells may furthermore be part of a tissue, an organ or a complete organism such as a plant or an animal. The cells may be in a naturally occurring form or in a man-made form such as in a cultured form, e.g. cell culture, protoplast culture, tissue culture or the like.

The term "derived" used in connection with characterizing the biological sample means any kind of measures a skilled person may apply in order to modify the labeled cells or the direct environment of the cells, wherein the "direct environment"

is characterized by the presence of at least one metabolite produced by the cells, in order to prepare a sample for use in quantitatively determining the metabolites contained therein by applying the method of the invention. Such measures may for example involve typical sample preparation or extraction techniques common to those skilled in the art. The direct environment may for example be the extracellular space around a cell, the apoplast, the cell wall, the interstitial space or the culture medium. Furthermore, the biological sample derived from a cell may be a certain part of the cell, for example certain cellular compartments such as plastids, mitochondria, the nucleus, vacuoles etc. In a preferred embodiment of the present invention, the biological sample comprises yeast cells or plant cells.

A "biological sample" in the context of the present invention can for instance be fresh material such as a tissue explant, a body fluid or an aliquot from a bacterial or cell culture, preferably deprived of the culture medium, that may be directly subjected to extraction. On the other hand, samples may also be stored for a certain time period, preferably in a form that prevents degradation of the metabolites in the sample. For this purpose, the sample may be frozen, for instance in liquid nitrogen, or lyophilized. The samples may be prepared according to methods known to the person skilled in the art and as described in the literature. In particular, the preparation should be carried out in a way suitable to the respective detection technique applied. Furthermore, care should be taken that the respective compounds to be analyzed are not degraded during the extraction process. Biological samples for metabolite analyses may for example be prepared according to procedures described in Roessner (2000).

In a further preferred embodiment, the method of the invention further comprises fractionating or purifying the biological sample so that the sample contains a subset of the metabolites contained in the cell from which the sample is derived.

By this additional fractionation and/or purification step, it is for example possible to select low abundant metabolites out of the whole pool of metabolites whereby, without this step, these metabolites might not be detectable for example because their signals are superimposed with strong signals of highly abundant metabolites. In prior art metabolite profiling methods, such a fractionation or purification would cause the loss of the quantitative relationship to other metabolites which would render the

quantification of low abundant metabolites nearly impossible. This problem has been overcome by the present invention since the isotopically labeled metabolites serve as a quantitative standard that may be co-fractionated/-purified with the non-labeled metabolites.

The fractionation and/or purification may be carried out according to standard procedures known in the art. It is clear that preferably procedures should be used that do not or at least only to a low tolerable degree change the distribution of the metabolites in the sample.

The quantitative determination of metabolites in a biological sample may be carried out by any known suitable method that can resolve mass differences within one metabolite. This may involve various nuclear magnet resonance (NMR) and mass spectrometry (MS) techniques that are known to a person skilled in the art, whereby mass spectrometry is preferred in the context of the present invention. Different suitable NMR and MS techniques are for instance described in Wittmann (Adv. Biochem. Engin. Biotechnol. 74 (2002), 39-64) and Szyperski (Q. Rev. Biophys. 31 (1998), 41-106). Preferred set ups for MS techniques for use in the present invention involve the combination of MS with gas chromatography (GC) as it is routinely used in state-of-the-art metabolite analyses, such as GC-MS described in the appended Examples.

In cases of ambiguous fragment interpretation, analyses using GC-MS-MS or corresponding MS tandem arrangements may support the identification of isotopomer fragment pairs. For example, GC-MS systems supplied with ion trap technology allow the selection of individual primary fragments and subsequent secondary mass spectral fragmentation (Birkemeyer, 2003; Mueller, 2002). These MS-MS mass spectral fingerprints may allow an unequivocal identification of corresponding primary ions.

The determination of the amount of metabolites of interest can be done according to well-known techniques known in the prior art and familiar to the person skilled in the art. Preferably, techniques are applied that allow the identification and quantification in one step and, advantageously, are suited to record the respective metabolites contained in the sample in a comprehensive manner.

Further methods for quantitatively determining the metabolites for use in accordance in the present invention include liquid chromatography/mass spectrometry (LC/MS), the use of radioactivity in connection with suitable methods known to the skilled person, thin layer chromatography (TLC), capillary electrophoresis (CE), direct injection MS, flow injection MS, MS/MS, MS/MS/MS, and further combinations of MS steps (MS<sub>n</sub>), fourier transform ion mass spectrometry (FT/MS), gel permeation chromatography (GPC), TLC, CE, HPLC, GPC, any other chromatographic or electrophoretic technique or any mass spectrometric technique which is hyphenated in-line or off-line to mass spectrometry. If appropriate, any of the above methods may be combined.

An exemplary non-biased analyses is described in Fiehn (2000b). In this study, of different plant mutants, 326 distinct compounds (ranging from primary polar metabolites to sterols) were detected and relatively quantified, including both identified and non-identified compounds, by applying GC/MS analyses. Another example of a GC/MS analyses that can be applied in the method of the invention has been described by Roessner (2001), where it was used for comprehensively studying the metabolism in potato tubers.

In a particularly preferred embodiment of the method of the invention, the mass spectrometry used is matrix-assisted laser desorption ionisation/time-of-flight (MALDI-TOF) mass spectrometry.

This embodiment makes use of the surprising finding that the saturating in vivo labeling achieved by the method of the invention makes it possible to obtain quantitative metabolite profile data.

It is furthermore preferred that the method of the invention as described hereinabove involves that the metabolites are chromatographically separated prior to quantitative determination.

This preferred embodiment refers to the chromatographic separation which has already been described above by referring to the particularly preferred example of using gas chromatography in settings such as GC-MS or GC-MS-MS. Other suitable chromatography methods such as HPLC, RP-HPLC, ion-exchange HPLC, GPC, capillary electrophoresis, electrophoresis, TLC, chip-base micro-fluidic separation,

affinity-interaction chromatography using antibodies or other ligand-specific binding domains may also be used in this regard.

In another preferred embodiment, the method of the invention further comprises the step of introducing external standards for one or more of the quantitatively determined metabolites.

The introduction of external standards or standard dilution series allows the determination of metabolite concentrations in absolute terms. By contrast, embodiments of the method of the invention in which no external standards or standard dilution series are applied allow the exact quantification in relative terms, i.e. concentration changes observed relative to reference quantities as observed in experimental control samples. The introduction of external standards and the provision of such standards may be carried out as described in the literature and as is known by the person skilled in the art.

As has been mentioned above, the method of the invention includes the quantitative determination of metabolites the chemical nature of which is yet unknown. Accordingly, in a preferred embodiment, this method further comprises the step of identifying one or more of the metabolites which are quantitatively determined.

This identification may be carried out by analytical methods known to the skilled practitioner and described in the literature.

In a particularly preferred embodiment, this identification comprises identification by secondary fragmentation.

Secondary fragmentation techniques may be carried out by methods known in the prior art; in particular by GC-MS-MS or other MS<sup>n</sup> techniques. Separate recording and subsequent comparison of chemical intermediates from MS-MS fragmentation pathways of, e.g., <sup>13</sup>C isotopomer pairs is highly facilitated by providing the number of carbon atoms present within each observed MS-MS fragment.

In an especially preferred form of this embodiment, identification of the metabolites comprises electron impact ionisation, MS-MS technology and/or post source decay analyses of molecular ions or fragments.

Such techniques are known to a person skilled in the art. In particular, post source decay analyses may be carried out as is described in Example 9 using NADH detection as an example.

In a further preferred embodiment, the method of the invention as described above may be carried out in such a way that the cell to be labeled has been maintained under conditions additionally allowing the uptake of an isotopically unlabeled metabolizable compound and said compound and/or metabolic products thereof are quantitatively determined. Preferably, the uptake of the unlabeled compound takes place when the cell is already saturated with the isotopic label.

Preferably, this embodiment involves comparing the amount determined for the isotopically unlabeled metabolizable compound and/or said metabolic products thereof with the amount obtained by carrying out said method correspondingly, but without the uptake of said unlabeled metabolizable compound.

The present preferred embodiment relates to an application of the present invention which is also referred to as "inverse labeling". This term refers to an inversion of conventional flux studies (see, e.g., Wittmann, Adv. Biochem. Engin. Biotechnol. 74 (2002), 39-64) in which a labeled metabolite is added to a cell and its fate is traced in order to analyse metabolic pathways. The present preferred embodiment of the invention appears to be feasible because of the high similarity of metabolite profiles from ambient  $\delta^{13}\text{C}$ - and  $^{13}\text{C}$ -saturated yeast cultures (Figure 2 A, B). Moreover, in Example 2, a corresponding experiment is described in which L-lysine was added in unlabeled form to the culture medium after the yeast cells reached saturated  $^{13}\text{C}$ -labeling. In a further experiment, the enrichment of the non-labeled trace compound nicotinic acid and the incorporation of this moiety into NAD(H) within a  $^{13}\text{C}$ -saturated yeast metabolome was shown (Example 9).

The present embodiment allows it to achieve results similar to those obtained in conventional flux studies. It allows to utilize the relatively inexpensive supply of substances with ambient  $\delta^{13}\text{C}$  composition for biochemical pathway elucidation within the background of a  $^{13}\text{C}$ -saturated metabolome. But it has the advantage that the specific metabolite the metabolization of which shall be analysed does not need to be provided in labeled form, which often is considerably expensive. Rather, in the method according to the present embodiment, the metabolite to be investigated can



be used in the cheaper unlabeled form. A further advantage is the increased versatility of this approach as compared to conventional flux studies since virtually every possible metabolite can be tested for or even more than one metabolite, without being dependent on the availability of the metabolite(s) in labeled form.

In a further preferred embodiment of the above-described method of the invention, one or more proteins and/or transcripts in said sample(s) is/are quantitatively determined and analysed, in addition to metabolites.

This embodiment refers to one of the main aspects in systems biology which aims at combining metabolome data with data obtained from transcriptome and/or proteome analyses in order to obtain a comprehensive picture of regulatory mechanisms in biological systems. In this context, it is evident that the method of the present invention may be combined with methods that quantitatively determine transcripts and/or proteins from the same biological system, in particular organism or cells, of which the metabolites are quantitatively analysed in accordance with the method of the invention. Transcriptome and proteome analyses as well as mathematical evaluation and correlation analyses of the data may be conducted by methods described in the prior art. It is contemplated that, preferably, the transcriptome and/or proteome analyses conducted in combination with the metabolome analyses according to the present invention may also benefit from the advantages of in vivo labeling. Thus, if the quantitative determination of transcripts or proteins is done by suitable techniques such as mass spectrometry the transcripts or proteins may be isotopically labeled just as the metabolites and thereby also be used as a quantitative standard.

It is particularly preferred that the preferred embodiment is carried out in such a manner that said metabolites and proteins and/or transcripts are each determined from the same biological sample.

This particularly preferred embodiment is based on a technology described in WO 03/058238 and in Fiehn (Eur. J. Biochem. 270 (2003), 579-588). The method described therein provides data useful for quantitatively analyzing metabolites, proteins and/or RNA in a biological source material, whereby said analyses involves suitable statistical evaluation and correlation analyses on the data obtained. In this

method, extracting, identifying and quantifying of at least two compound classes of the group consisting of metabolites, proteins and RNA are each determined from one sample. Accordingly, in the present particularly preferred embodiment, the sample preparation in order to quantitatively determine metabolites and proteins and/or transcripts is carried out by applying the corresponding teachings of WO 03/058238. Thereby, it is especially preferred that (i) the metabolites are extracted from the sample with at least one solvent or mixture of solvents; and (ii) the RNA is extracted from the remainder of the sample after step (i). Thereby, it is a further option that metabolites may additionally be extracted from the yet undissolved remaining cellular material contained in the sample after step (ii). Preferably, extraction is carried out by using a mixture of solvents that comprises at least one highly polar solvent, at least one less polar solvent and at least one lipophilic solvent, advantageously a mixture of solvents comprising water, methanol and chloroform. More preferably, this mixture of solvents contains water, methanol and chloroform in the approximate proportion by volume of 1: 2.5: 1. Advantageously, the extraction in step (i) is carried out at a temperature between -60°C and +4°C.

As a further preferred embodiment of the present invention, the method as described hereinabove further comprises, prior to quantitative determining the metabolites, combining the biological sample (i.e. the first biological sample) with a second biological sample in which the metabolites are not isotopically labeled or are isotopically labeled differently from the first biological sample; and determining in said biological samples the relative quantity of metabolites which differ by their isotopical label.

Preferably, the second biological sample is not isotopically labeled.

By this preferred embodiment, the method facilitates the quantification of metabolite data which hitherto was only possible by using external metabolite samples as quantitative standards. Here, the in vivo labeled metabolites present the quantitative standard for the metabolites of the second biological sample. This allows the correlation analyses of a wide set of metabolites of two biological samples which correspond to two different phenotypic and/or genotypic states of the cells from which the biological samples are derived.

Accordingly, in a specifically preferred embodiment, the first and the second biological sample correspond to different phenotypic and/or genotypic states of the cells comprised in the samples or from which the samples are derived.

By applying this embodiment of the method of the invention, it is possible to find correlations between the difference in the phenotypic and/or genotypic state and changes in the metabolite profile for instance by performing metabolite co-response analyses.

The term "phenotypic state" refers to differences in the phenotype of the cell under investigation or the organism in which it resides. "Phenotype" means any kind of feature that can be detected and which is not a feature of the genome. Such phenotypic states may for example be visually identifiable such as a morphological or anatomical difference like they can be observed at different developmental stages. Phenotypic states may likewise manifest themselves by the composition of chemical compounds or the occurrence of a disease. Thus, the phenotypic states may for instance be a healthy state in comparison to one or more pathogenic states, different stages of a pathogenicity or an uninfected versus one or more infected organisms.

The term "genotypic state" reflects differences in the genome of the cells under investigation. Thus, if the samples are taken from different genotypic states of a cell, the term "cell" specifically refers to cells according to the definition given above which belong to the same taxonomic unit, but which differ in at least one genetic trait. Specifically, the "taxonomic unit" is a genus, preferably a species, and more preferably an even lower taxonomic rank such as a race, variety, cultivar, strain, isolate, population or the like. Most preferably, the taxonomic rank is an isogenic line with variance in only a limited number, preferably three, more preferably two genetic traits and most preferably one genetic trait, whereby "genetic trait" refers to a chromosomal region, a gene locus or, as it is preferred, to a gene. Typically, differences in the genotypic state can be differences between a wild-type organism and one or more corresponding mutant or transgenic organisms or between different mutant or transgenic organisms. A certain genotypic state may be stable or transient as is the case with transduced or transfected cells, for instance containing a plasmid, phage or viral vector. Advantageously, organisms of different genotypic state are analyzed when they are in the same developmental stage.

It is immediately clear that the terms "phenotypic" and "genotypic" states may overlap. In particular, normally a genotypic state, if the differing genetic trait(s) is/are expressed in the organism, lead(s) to a difference in the phenotype.

According to the above explanations, in a preferred embodiment of the method of the invention, the different phenotypic and/or genotypic states are different developmental stages, environments, nutritional supplies, taxonomic units, wild-type and mutant or transgenic genomes, infected and uninfected states, diseased and healthy states or different stages of a pathogenicity.

In a further preferred embodiment of the method of the invention as described hereinabove, said analysing further involves suitable statistical evaluation and correlation analyses of the data obtained and, optionally, network analyses.

This refers to any mathematical analyses method that is suited to further process the quantitative data provided by the method of the invention. This data represents the amount of the analyzed metabolites present in each sample either in absolute terms (e.g. weight or moles per weight sample) or in relative terms (i.e. normalized to a certain reference quantity).

Quantitative analyses involves suitable statistical evaluation and correlation analyses. The former includes normalization to the total content of the respective compounds, correction of background levels and the combination of the data sets obtained from different experiments (if more than one sample is analysed) into a single data sheet. Corresponding mathematical methods and computer programs are known to the skilled practitioner. Examples include SAS, SPSS and systatR. As the next step, the statistically pre-treated data may be subjected to a pairwise correlation analyses. Here series of pairs of data points from the analyzed compounds are looked at for correlation, whether positive or negative, for instance using Pearson's correlation coefficient.

In a preferred embodiment, the quantitative analyses referred to in the method of the invention furthermore involves network analyses. Network analyses aims at finding out higher order interplays of multiple factors on the basis of pairwise correlation data. If, according to one of the above-described preferred embodiments, metabolites and transcripts and/or proteins are quantitatively determined, for the obtained several

data sets, preferably each obtained from one sample, correlations between metabolites and proteins and/or transcripts as well as within these classes of compounds can be analyzed in order to derive information about the network regulation of biological systems, e.g. upon genetic or environmental perturbation. A comprehensive overview of methods for quantitatively analyzing data obtained according to the method of the invention including principle component analyses, "snapshot analyses", Pearson correlation analyses, mutual information and network analyses can be found in Fiehn (2001).

In a further aspect, the present invention relates to a set of isotopically labeled metabolites obtainable from a sample which comprises or is derived from a cell which has been maintained under conditions allowing the uptake of an isotopically labeled metabolizable compound so that the metabolites in said cell are saturated with the isotope with which said metabolizable compound is labeled.

The present invention also relates to such cells which can be cells as described above in connection with the method of the invention.

As is explained hereinbefore, the isotopically labeled metabolites obtained from a biological sample in accordance with the method of the present invention may be used as a quantitative standard for the quantitative determination of the metabolites of a second biological sample. Thus, a set of these labeled metabolites is also an object of the present invention. Preferably, this set can be used to standardize results of a metabolome analyses conducted with the same species of cells as that from which the set of metabolites is obtained. However, it is also feasible that this set may be of use to standardize metabolite data obtained from a different species. This would generally require that metabolites of the set are identical with metabolites of the second biological sample. Identity can be determined or confirmed by using methods known in the art and described herein. For instance, the in vivo isotopically labeled metabolites obtained from yeast may be used as a quantitative standard for metabolites of plant cells since, for a considerable subset of each of these metabolites, the metabolites overlap such as the metabolites of the primary metabolic pathways.

As a further use of the set of isotopically labeled metabolites of the invention, or corresponding cells containing them, it is envisaged that the set or the cells can be

used as a qualitative standard in order to identify metabolites from a second, unlabeled biological sample.

The set of metabolites may be prepared in accordance with the above explanations for carrying out the method of the invention. For the purposes of storing and transporting that set, corresponding methods may be applied which are suitable in order to ensure that degradation of each kind of metabolite contained therein is at least minimized to a tolerable degree and which are known to a person skilled in the art.

In a further embodiment, the present invention refers to the use of the set of isotopically labeled metabolites mentioned above as a quantitative standard for determining the amount of one or more metabolites in a biological sample.

Furthermore, the present invention relates to a kit comprising an isotopically labeled metabolizable compound and a manual for use in carrying in out the method of the invention or the set of isotopically labeled metabolites described above.

The components of the kit of the invention may be packaged in containers such as vials in a storable and transportable form. If appropriate, one or more of said components may be packaged in one and the same container.

Additionally, the present invention relates to the use of an isotopically labeled compound that can be metabolized by a cell for labeling the metabolites in said cell in a saturating manner.

Such uses may be carried out in accordance with the above-outlined explanations for the method of the invention.

The present invention also relates to the use of an isotopically labeled compound that can be metabolized by a cell for the quantitative determination of metabolites in a biological sample comprising or being derived from said cell.

Such uses may be carried out in accordance with the above-outlined explanations for the method of the invention.

Likewise, the present invention relates to the use of an isotopically labeled compound that can be metabolized by a cell for analysing the metabolite profile of a biological sample comprising or being derived from said cell.

Such uses may be carried out in accordance with the above-outlined explanations for the method of the invention.

These and other embodiments are disclosed and encompassed by the description and examples of the present invention. All of the publications, patents and patent applications referred to in the specification in order to illustrate the invention are hereby incorporated by the reference in their entirety. Further literature concerning any one of the methods, uses and compounds to be employed in accordance with the present invention may be retrieved from public libraries, using for example electronic devices. For example the public database "Medline" may be utilized which is available on the Internet, for example under <http://www.ncbi.nlm.nih.gov/PubMed/medline.html>. Further databases and addresses, such as <http://www.ncbi.nlm.nih.gov/>, <http://www.infobiogen.fr/>, [http://www.fmi.ch/biology/research\\_tools.html](http://www.fmi.ch/biology/research_tools.html), <http://www.tigr.org/>, are known to the person skilled in the art and can also be obtained using, e.g., <http://www.google.de>. An overview of patent information in biotechnology and a survey of relevant sources of patent information useful for retrospective searching and for current awareness is given in Berks, TIBTECH 12 (1994), 352-364.

Furthermore, the term "and/or" when occurring herein includes the meaning of "and", "or" and "all or any other combination of the elements connected by said term".

The present invention is further described by reference to the following non-limiting figures, tables and examples.

The Figures and the Tables show:

**Figure 1** shows the results of head-to-tail analyses of electron impact ionisation mass spectra of yeast metabolites extracted from GC-MS metabolite profiles.

The yeast metabolites succinic acid, glycine and glutamic acid were trimethylsilylated prior to GC analyses. The number of silylated functional groups and the magnification factor of the high molecular mass range is indicated. Head-to-tail mass spectra are from separate GC-MS analyses of ambient  $\delta^{13}\text{C}$ - and  $^{13}\text{C}$ -saturated yeast extracts. Insets to the right show the  $\text{M}^+$  and  $[\text{M}-15]^+$  fragment ranges of combined  $^{13}\text{C}$ -isotopomer ratio (ITR) metabolite profiles. The isotopomer  $[\text{M}-15]^+$  fragment pairs of succinic acid (2TMS), glycine (3TMS), and glutamic acid (3TMS) are  $\text{M/Z}$  247\_251,  $\text{M/Z}$  276\_278, and  $\text{M/Z}$  348\_353. Glutamic acid (3TMS) exhibited abundant molecular ions,  $\text{M}^+$ ,  $\text{M/Z}$  363\_368.

**Figure 2** depicts a comparison of ITR metabolite profiling (A, C) and conventional metabolite profiling (B,D).

Selected ion responses of  $^{12}\text{C}$ - and  $^{13}\text{C}$ -isotopomer fragment pairs, which represent the same substance from ambient  $\delta^{13}\text{C}$ - and  $^{13}\text{C}$ -saturated yeast extracts (A, B), and fragments which represent the same isotopomer in two different experiments (Exp1 and Exp2) from either the ambient  $\delta^{13}\text{C}$ - or  $^{13}\text{C}$ -saturated yeast culture (C, D) are plotted. ITR was performed in two GC-MS analyses (06, 10), whereas four GC-MS analyses were required for conventional metabolite profiling (ambient  $\delta^{13}\text{C}$ : 04, 08;  $^{13}\text{C}$ -saturated: 05, 09). Pearson's linear correlation coefficients ( $r$ ) and average coefficients of variation ( $cf$ ) are shown in the insets.

**Figure 3** represents a GC-TOF-MS metabolite profile of yeast strain BY4741.

Ticks below the total ion current trace of the main profile indicate the automated deconvolution of mass spectral components with  $\text{S/N} \geq 100$  which were performed by Pegasus chromatography data processing software. The inset shows selected ion traces of deconvoluted components from the shaded area of the main profile. **A** isoleucine (2TMS),  $\text{M/Z} = 158$ ; **B** threonine (2TMS),  $\text{M/Z} = 117$ ; **C** proline (2TMS),



M/Z = 142; D glycine (3TMS), M/Z = 174; E 2,2,3,3-d4-succinic acid (2TMS), M/Z = 251; F succinic acid (2TMS); M/Z = 247 (factor of magnification 10). The presence of 2,2,3,3-d4-succinic acid resulted from standard addition of a deuterated isotopomer.

**Figure 4** depicts a clustering tree of identified, and non-identified MSTs from extracts of *Saccharomyces cerevisiae* strain BY4741 and pure standard compounds. MSTs were classified into groups by hierarchical clustering of a complete symmetric matrix of pair-wise mass spectral match values (Table 4). 18 groups of MSTs were classified at a cut-off at approximately 50 % diversity (the MST groups are described in Example 6).

**Figure 5** shows the results of a principal component analyses based on GC-TOF-MS metabolite profiles of extracts from a single batch culture of *Saccharomyces cerevisiae* strain BY4741 ( $A_{595} \sim 1.8$ ). Four sampling strategies ( $n = 16$ ) were employed, namely quenching into cold methanol (MEOH), collection onto filter disc (FILTER), collection by centrifugation without media wash (SPIN), and collection by repeated wash and centrifugation cycles (SPINW). Washes were performed with glucose-free SD medium. Principal components 1, 2, and 3 covered 57.4 %, 24.2 %, and 6.4 % of the total variance of the profile data set. Metabolite responses were normalised to the average metabolite response observed within each sample. Average relative standard deviation (RSD) of each of the sampling procedures is indicated. Underlying metabolite profiles, metabolite responses and relative standard deviations of all metabolites are presented in Table 6.

**Figure 6** provides the results of a comparison of four co-response measures applied to metabolite profiles of *Saccharomyces cerevisiae* strain BY4741 ( $A_{595} \sim 1.8$ ). Kendall's correlation coefficient is compared to Euclidian distance (A), mutual information (B) and Pearson's correlation coefficient (C). Each tuple represents a metabolite/metabolite co-

response. Arrows indicate position of exemplary bi-plots presented in double-log<sub>10</sub> scale to the right. Four sampling strategies ( $n = 16$ ) were employed, namely MEOH, FILTER, SPIN, and SPINW. The sampling techniques were as described within the legend to Figure 5. A complete overview of all pair-wise metabolite/metabolite co-response measures is given in Table 7.

**Figure 7** shows metabolite bi-plots in double-log<sub>10</sub> scale representing co-response behaviour of intermediates and a product of the tricarboxylic acid cycle. Oxaloacetic acid was below limits of detection in GC-TOF-MS profiles of yeast. **A**, malic acid/ aspartic acid; **B**, malic acid/ citric acid; **C**, fumaric acid/ malic acid; **D**, succinic acid/ fumaric acid. The sampling techniques are as described within the legend to Figure 5.

**Figure 8** shows the common nearest and most distant neighbours of succinic acid, fumaric acid, and malic acid, as described by Kendall's correlation coefficient. Values of correlation coefficients were coded by line style,  $\geq 0.6$  full line and  $\leq -0.5$  dotted line.

**Figure 9** shows a continuous positive-ion MALDI-TOF-MS spectrum of an ambient  $\delta^{13}\text{C}$ -yeast extract with 2,5-dihydroxybenzoic acid as matrix set to the expected mass range of  $\text{NAD}^+$  ( $\text{NADH}$ ) adducts, namely protonated molecular ions at  $m/z$  664.11 (666.13), and sodium adducts at  $m/z$  686.09 (688.12), respectively. The inset ( $^{12}\text{C}/^{13}\text{C}$ ) shows a bar representation of the protonated molecular ion region from a  $^{13}\text{C}$ -isotopomer ratio ( $^{13}\text{C}$ -ITR) MALDI-TOF-MS analyses.  $m/z$  679.26 and 681.25 represent protonated  $\text{NAD}^+$  and  $\text{NADH}$ , which were labeled with 15  $^{13}\text{C}$ -atoms.  $^{13}\text{C}$ -saturated yeast extracts exclusively showed the labeled ions in the  $m/z$  677 - 685 range (data not shown).

**Figure 10** depicts a head-to-tail analyses of post source decay (PSD) fingerprints from separate MALDI-TOF-MS analyses of ambient  $\delta^{13}\text{C}$ - ( $^{12}\text{C}$  PSD) and  $^{13}\text{C}$ -saturated ( $^{13}\text{C}$  PSD) yeast extracts. Evident  $m/z$  differences of

parent ions and fragments were 15, 10, and 5 amu. The required mass window for the isolation of parent ions ( $\sim \pm 3$  amu) and subsequent PSD analyses did not allow separate monitoring of  $\text{NAD}^+$  and NADH from mixtures.

The following Examples illustrate the invention:

## **Experimental set-up**

### Strain information and in-vivo labeling

*Saccharomyces cerevisiae* strains BY4741 (MATa; his3 $\Delta$ 1; leu2 $\Delta$ 0; met15 $\Delta$ 0; ura3 $\Delta$ 0) and BY4742 (MAT $\alpha$ ; his3 $\Delta$ 1; leu2 $\Delta$ 0; lys2 $\Delta$ 0; ura3 $\Delta$ 0) were obtained from the EUROFAN II worldwide gene deletion project (EUROSCARF collection, Frankfurt, Germany. [http://www.uni-frankfurt.de/fb15/mikro/euroscarf/col\\_index.html](http://www.uni-frankfurt.de/fb15/mikro/euroscarf/col_index.html)) (Kelly, 2001; Winzeler, 1999). Strains were grown for 16-24 h in 25 - 250 ml liquid batch cultures on synthetic defined (SD) minimal medium with required auxotrophic supplementation and 20 g l<sup>-1</sup> ambient  $\delta^{13}\text{C}$ -glucose as major carbon source (Castrillo, 2003). For in-vivo  $^{13}\text{C}$ -labeling ambient glucose was replaced by U- $^{13}\text{C}$ -glucose (99 atom %, Isotech Inc., Miamisburg, USA). Auxotrophic and vitamin supplements were non-labeled.

For the control of residual SD medium components within cellular preparations from yeast cultures the media contained 4 g l<sup>-1</sup> lactose ( $\beta$ -D-galactopyranosyl-(1,4)-D-glucose, Fluka, Buchs, Switzerland), which is not utilized by *Saccharomyces cerevisiae*.

### Cellular preparations from yeast cultures

For all experiments 5 ml aliquots were taken from over-night yeast batch cultures grown to  $A_{595} \sim 1.8$ . Sampling procedures were: (1) MeOH, quenching into  $-50^\circ\text{C}$  cold methanol, subsequent centrifugation, and aspiration of supernatant (MeOH) (Castrillo, 2003; Gonzalez, 1997) with non-buffered quenching solution (see below);

(2) FILTER, vacuum collection onto 0.65  $\mu\text{m}$  Durapore PVDF hydrophilic membrane filter discs (Millipore GmbH, Schwalbach, Germany); (3) SPIN, collection by gentle centrifugation and complete aspiration of supernatant without subsequent wash; (4) SPINW, collection by 2 repeated gentle centrifugation and wash cycles with carbohydrate-free SD media. All procedures were performed at 28°C if not mentioned otherwise. Cellular preparations were either immediately processed or shock frozen in liquid nitrogen. Routine sampling was MEOH, if not indicated otherwise. As monitored by the lactose-tracer molecule all sampling methods except SPINW contained low amounts of residual media components. Non-sample control experiments with fresh SD media and analyses of the initial cell free medium and at time of sampling were performed (data not shown).

#### Preparation of intracellular yeast metabolites

Hot methanol/ chloroform extraction (15 min at 70°C), liquid phase partitioning into methanol/water (1:1, v/v), drying by vacuum centrifugation, and subsequent treatment with methoxyamine hydrochloride (MEOX) and N-methyl-N-(trimethylsilyl)-trifluoroacetamide (MSTFA) reagents for conventional yeast metabolite profiling of polar soluble material was down-scaled as described previously (Wagner, 2003). For the extended GC-TOF-MS analyses of yeast samples liquid partitioning by addition of water to the initial methanol/ chloroform extract was omitted. Instead the complete extract volume, ~ 700  $\mu\text{l}$ , was dried by vacuum centrifugation.

Supplementation of quenching- or extraction-solution with recommended buffer systems (Castrillo, 2003; Gonzalez, 1997) for the preparation of intracellular yeast metabolites led to strong interferences of the buffer substances with either methoxyamination, silylation, or chromatographic performance of the final sample preparations. Therefore, buffering substances had to be avoided for GC-MS profiling.

#### $^{13}\text{C}$ -isotopomer ratio (ITR) metabolite profiling

Extracts of intracellular yeast metabolites from ambient  $\delta^{13}\text{C}$ - and  $^{13}\text{C}$ -saturated cultures were combined in equal amounts prior to vacuum centrifugation. The  $^{13}\text{C}$ -

saturated extract was treated as a stable isotope labeled, multiplex internal standard mixture. Each component of the resulting metabolite profiles was quantified by use of the respective  $^{13}\text{C}$ -saturated compound. For this purpose  $^{12}\text{C}/^{13}\text{C}$  response ratios of pre-selected isotopomer fragment pairs were calculated (Table 2). Specific isotopomer fragment pairs were assigned manually to each identified and non-identified metabolite using respective mass spectral entries from the collection of mass spectral metabolite tags (MSTs; see below). Prior to forming ratios responses of  $^{13}\text{C}$ -saturated fragments were corrected for the contribution of naturally occurring  $^{13}\text{C}$ -isotopomers to ambient  $\delta^{13}\text{C}$ -preparations.

#### GC-MS technologies

Conventional GC-MS profiles were performed with a quadrupole type GC-MS system, namely a GC8000 gas chromatograph coupled to a Voyager mass spectrometer, which was operated by MassLab software (ThermoQuest, Manchester, UK). Modifications to the initial GC-MS profiling method (Fiehn, 2000a; Fiehn, 2000b) were, injection of 1  $\mu\text{l}$  sample in splitless mode, use of a  $5^\circ\text{C min}^{-1}$  temperature ramp with final temperature set to  $350^\circ\text{C}$  on a 30 m x 0.25 mm inner diameter Rtx-5Sil MS capillary column with an integrated guard column (Restek GmbH, Bad Homburg, Germany), and use of alkane mixtures for the determination of retention time indices. These changes reflect recent optimisation which was performed with a GC-TOF-Pegasus II MS system (Leco, St. Joseph, USA). All GC-TOF-MS experiments were done on a Pegasus II TOF-MS system as detailed earlier for a diverse range of plant samples (Wagner, 2003)

#### MALDI-TOF-MS technologies

Yeast extracts were analysed by MALDI-TOF-MS (Voyager DE-PRO Biospectrometry Workstation, Applied Biosystems, Foster City, USA) set to positive ion detection in reflectron mode (Lerouxel, 2002). Settings for reflectron MALDI-TOF-MS and PSD were as recommended by the manufacturer. A 2,5-dihydroxybenzoic acid ( $10 \text{ mg ml}^{-1}$ ) matrix was mixed 1:1 (v/v) with polar fractions from yeast extracts

or pure compounds, which were dissolved in methanol: water (1:1, v/v). Slow crystallisation by air drying was essential for the laser desorption and ionisation of  $\text{NAD}^+$  and  $\text{NADH}$ ; microcrystalline samples exhibited complete signal suppression. An exemplary study using the same MALDI-TOF-MS matrix previously demonstrated that stable isotope standardized MALDI-TOF-MS exhibited precise standard curves over two orders of magnitude and produced quantitative results in accordance with in-parallel gas chromatographic analyses (Kang, 2001).

#### Generation of a compendium MST library

MSTs (Table 3) were obtained through automated deconvolution of GC-TOF-MS chromatograms (ChromaTOF™ software, LECO, St. Joseph, USA). Mass spectra were collected into user libraries provided by NIST98 and AMDIS software ([http://chemdata.nist.gov/mass-spc/Srch\\_v1.7/index.html](http://chemdata.nist.gov/mass-spc/Srch_v1.7/index.html) and <http://chemdata.nist.gov/mass-spc/amdis/>; National Institute of Standards and Technology, Gaithersburg, USA) (Stein, 1999; Ausloos, 1999). MSTs were manually annotated and corrected for obvious errors caused by automated deconvolution. Mass spectra of low intensity and truncated or fused mass spectra which resulted from co-elution of compounds were rejected except for demonstrating of the presence of a labeled isotopomer.

#### Identification and classification of mass spectral metabolite tags (MSTs)

MSTs were identified by manually supervised standard addition experiments with pure commercially available substances. Required criteria for substance identification were chromatographic co-elution and high mass spectral similarity of MSTs observed within yeast samples to standard substances (Wagner, 2003). Co-elution and similarity were described by retention time index and mass spectral match values, respectively. Non-identified MSTs were tentatively analysed by best match with a customised MS library of standard substances and entries from the commercial NIST98 library (National Institute of Standards and Technology, Gaithersburg, USA). MSTs were classified by agglomerative hierarchical cluster analyses using Euclidian

distance measure and average linkage (Table 5, Figure 4). Cluster analyses was applied to a complete matrix of pair-wise mass spectral match values (Table 4) as described earlier (Wagner, 2003). Yeast MSTs and a selection of EI-TOF mass spectra from pure standard substances were co-classified.

#### Statistical analyses and visualisation of metabolite profiles

Principal component analyses (PCA), hierarchical clustering, calculation of Euclidian distance, Pearson's and Kendall's correlation coefficient, and mutual information was calculated using the S-Plus 2000 software package standard edition release 3 (Insightful, Berlin Germany), the programming language R version 1.6.1 and 1.6.2 (<http://www.r-project.org>) and the MetaGeneAlyse version 1.3 world wide web resource (<http://metagenealyse.mpimp-golm.mpg.de/>) (Daub, 2003).

The model for metabolic network representation was as suggested (Jeong, 2000) and overlay of correlation coefficients in accordance with modularity analyses in metabolic networks (Ravasz, 2002). Network visualisation and layout was performed using the Pajek (Batagelj, 1998) algorithm package available at <http://vlado.fmf.uni-lj.si/pub/networks/pajek/>.

#### Calculation of metabolite profiles

Each metabolite was represented by a single response value (Table 6). Within GC-MS profiles single metabolites may be represented by multiple derivatives, which are detected by respective MSTs, and each MSTs may be represented by more than one specific fragment (refer to Table 2 and Figure 1). In these cases an additive composite metabolite response was calculated rather than selecting a single MST and corresponding fragment.

Metabolite response was normalised to the average signal intensity of all MSTs, which were observed within each single GC-MS chromatogram. This strategy of data normalisation was mandatory prior to comparison of sampling technologies and analyses of metabolite co-response, because sampling technologies had variable and different recoveries of viable cells from the same batch culture. For example,

each wash cycle of SPINW sampling successively reduced recovery of viable cells (data not shown). Attempts failed to identify a constitutive metabolite, which would allow to exactly monitor the number and size of viable yeast cells within each preparation.

### **Example 1: Determination of the extent of saturation by in vivo $^{13}\text{C}$ -labeling**

In order to determine the completeness of in vivo  $^{13}\text{C}$ -labeling (saturation), yeast cells (yeast strain BY 4741; Kelly, 2001; Winzeler, 1999) were fed with U- $^{13}\text{C}$ -glucose as the only carbon source except for auxotrophic and vitamin supplements, i.e. biotin, pantothenate, folic acid, inositol, niacin, p-aminobenzoic acid, pyridoxine, riboflavin, thiamine, bacto-yeast nitrogen base without amino acids, histidine, leucine, methionine, uracil, and inorganic salts, i.e. ammonium sulfate, boric acid, copper sulfate, potassium iodide, ferric chloride, manganese sulfate, sodium molybdate, zinc sulfate, potassium phosphate, magnesium sulfate, sodium chloride, calcium chloride that were non-labeled and extracts from these yeast cells were examined by conventional electron impact GC-MS for the content of different metabolites. As judged by the resulting mass spectra profiles, the majority of the detectable metabolites from the yeast cells was completely labeled. In detail, ambient (i.e. naturally occurring)  $^{12}\text{C}/^{13}\text{C}$ -carbon ( $\delta^{13}\text{C}$ -) isotopomer composition was found for uracil, methionine, histidine, nicotinic acid and inositol in extracts prepared from cultures supplemented with U- $^{13}\text{C}$  glucose. Non-labeled leucine and pantothenic acid were frequently observed, however these metabolites were only abundant at levels close to detection limits. Other vitamins comprised by SD media, e.g. biotin, folic acid, p-aminobenzoic acid, pyridoxine, riboflavin, and thiamine, were below limits of detection or not accessible by GC-MS technology.

Furthermore, homocysteine, and inositol-phosphate were detected devoid of  $^{13}\text{C}$ -label. A still non-identified conjugate of inositol exhibiting high similarity to galactinol was partially labeled, and uridine carried 5 out of 9 possible  $^{13}\text{C}$  atoms. These findings indicate: (1) synthesis of homocysteine from methionine by 5-methyltetrahydropteroyltri-L-glutamate:L-homocysteine S-methyltransferase (EC 2.1.1.14; MET6), (2) a pathway from inositol to inositol-phosphate possibly through



phosphatidylinositol synthase (2.7.8.11; PIS) and phospholipase C (3.1.4.11; PLC1) activity, and (3) uracil scavenged by uracil phosphoribosyltransferase (EC 2.4.2.9; FUR1) and subsequent phosphatase action.

### **Example 2: "Inverse labeling" of yeast cells**

L-lysine supplementation of yeast strain BY 4741 was tested in  $^{13}\text{C}$ -saturated cultures. Lysine is the complementary auxotrophic marker substance of the second *Saccharomyces cerevisiae* strain BY4742 used by the EUROFAN II worldwide gene deletion project (Kelly, 2001; Winzeler, 1999).  $^{13}\text{C}$ -labeling of lysine was suppressed in strain BY4741 when supplemented with this amino acid. Moreover, 2-aminoadipic acid accumulated only in strain BY4742. This results indicates that the bi-directional L-lysine synthesis and degradation pathway which comprises the activities of L-aminoadipate-semialdehyde dehydrogenase (EC 1.2.1.31; LYS2, LYS5),  $\text{NADP}^+$ , L-glutamate-forming saccharopine dehydrogenase (EC 1.5.1.10; LYS9), and  $\text{NAD}^+$ , L-lysine-forming saccharopine dehydrogenase (EC 1.5.1.7; LYS1) is interrupted.

### **Example 3: Identification of $^{12}\text{C}$ - and $^{13}\text{C}$ -isotopomer pairs**

Reliable identification of pairs of  $^{12}\text{C}$ - and  $^{13}\text{C}$ -isotopomers which represent the same metabolite is a prerequisite for accurate isotopomers ratio (ITR) metabolite profiles. Pairs of isotopomers may be identified based on mass spectral fragmentation as well as by chromatographic retention. Initial GC-MS experiments demonstrated that derivatives of commercially available deuterated compounds had significantly smaller retention time indices (RI) than non-deuterated compounds. For example, 2,3,3,3-D<sub>4</sub> alanine (2 TMS), 2,3,3-D<sub>3</sub>-aspartic acid (3 TMS), 2,3,3,3-D<sub>4</sub> alanine (3 TMS), 2,2,3,3-D<sub>4</sub>-succinic acid (2 TMS), and 2,3,4,4,4,5,5,5-D<sub>8</sub>- valine (2 TMS) eluted 1.1, 1.8, 2.3, 2.5, and 3.8 RI units prior to respective non-deuterated isotopomers.

In contrast, commercially available  $^{13}\text{C}$ -labeled compounds exhibited only minor shifts in RI. This observation was confirmed by a selection of 66  $^{13}\text{C}$ -labeled mass spectral metabolite tags (MSTs) observed in standard GC-MS profiles. This testing set of MSTs was selected according to high mass spectral peak purity and presence

of at least one abundant and specific fragment which could be employed for selective ion quantification and RI monitoring. The selection comprised derivatives of amino acids, organic acids, sugars, sugar alcohols, sugar phosphates, and a set of 34 non-identified MSTs. The complete list including all available and manually evaluated GC-EI-MS isotopomer fragment pairs is listed in Table 2 (see *infra*). RI of  $^{13}\text{C}$ -labeled compounds was on average only 0.28 ( $\pm 0.53$  SD) units smaller than those of non-labeled compounds. This slight shift of RI was equivalent to approximately 0.3 sec of retention time.

Interpretation of the EI-MS fragmentation pattern of pairs of ambient  $\delta^{13}\text{C}$ - and  $^{13}\text{C}$ -isotopomers allowed the verification of metabolite identity. Typical EI mass spectra of succinic acid (2 TMS), glycine (3 TMS), and glutamic acid (3TMS), are shown in Figure 1. The head to tail analyses of ambient  $\delta^{13}\text{C}$ - and  $^{13}\text{C}$ -EI-mass spectra allowed an easy identification of isotopomer fragment pairs for use in ITR metabolic profiling. For example, glutamic acid ( $\text{C}_5\text{H}_9\text{NO}_4$ ) forms a TMS derivative with the sum formula  $\text{C}_{14}\text{H}_{33}\text{NO}_4\text{Si}_3$  and a relative molecular mass of 363. The molecular ion  $\text{M}^+$ ,  $m/z$  363, and the  $[\text{M}-15]^+$  fragment,  $m/z$  348, which is generated by typical neutral loss of a  $\text{CH}_3$ -radical from a TMS group, correspond to ions being characterized by  $m/z$  368 and  $m/z$  353 in which all 5 carbon atoms of glutamic acid are  $^{13}\text{C}$ -labeled. The fragment  $[\text{M}-117]^+$ ,  $m/z$  246, can be matched with the corresponding  $^{13}\text{C}$ -isotopomer fragment,  $m/z$  250. These fragments are formed by neutral loss of a trimethylsilylated carboxyl group, which contains one of the 5 carbon atoms of the glutamic acid. The  $\text{M}^+$  and  $[\text{M}-15]^+$  fragments of ambient  $\delta^{13}\text{C}$ - and  $^{13}\text{C}$ -saturated succinic acid (2 TMS), glycine (3 TMS) and glutamic acid (3TMS) are shown in the insets of Figure 1. These mixed mass spectra were obtained from  $^{13}\text{C}$ -ITR metabolite profiles, i.e. combined analyses of ambient  $\delta^{13}\text{C}$ - and  $^{13}\text{C}$ -saturated yeast extracts within single chromatograms. The chosen examples also demonstrate the necessity to correct  $^{13}\text{C}$ -ITR metabolite profiles for ambient  $^{13}\text{C}$ -isotopomer abundance, especially when the available mass spectral fragments for  $^{13}\text{C}$ -ITR metabolite profiles contain only 1 or 2 labeled carbon atoms.

**Example 4: Comparison of  $^{13}\text{C}$ -ITR metabolite profiles with conventionally produced metabolite profiles**

$^{13}\text{C}$ -ITR metabolite profiles produced by combining equal amounts of ambient  $\delta^{13}\text{C}$ - and  $^{13}\text{C}$ -saturated yeast extracts into one GC-MS analyses were compared with conventional, i.e. separate, GC-MS profiles of the same extracts. The above-mentioned testing set of yeast MSTs was used for this comparison. Each MST was quantified by up to 3 manually validated isotopomer fragment pairs Table 2 (see *infra*). This experiment was performed with the aim to establish whether ITR metabolite profiling which utilizes internal standardisation by each the  $^{13}\text{C}$ -labeled compounds is equivalent with conventional metabolite profiling. The latter approach was shown previously to operate successfully by external quantification (Fiehn, 2000a; Roessner, 2000).

Two yeast cultures were grown from the same colony in liquid SD medium. One culture was supplemented with ambient  $\delta^{13}\text{C}$ -glucose, the second with  $\text{U-}^{13}\text{C}$ -glucose. Extracts of these cultures were either analysed separately or combined for  $^{13}\text{C}$ -ITR before derivatisation. An initial experiment (Exp1) was repeated by taking a second sample from the same culture after a 15 min time interval (Exp2).

Two comparisons were performed based on the resulting metabolite profiles. (1) Comparison of Exp1 with Exp2 demonstrated the analytical variability, by means of re-analysing the same cultures (Figures 2C and 2D). (2) Comparison of the GC-MS responses of the labeled and non-labeled isotopomer fragment pairs showed the effect of  $^{13}\text{C}$ -saturation on metabolic profiles (Figures 2A and 2B). Both comparisons were done either by ITR metabolite profiling (Figures 2A and 2C; ITR GC-MS analyses 06 and 10) or by conventional metabolite profiling (Figures 2B and 2D; ambient  $\delta^{13}\text{C}$  GC-MS analyses 04 and 08;  $^{13}\text{C}$ -saturated GC-MS analyses 05 and 09). GC-MS analyses 04, 05 and 06 represented Exp1, while analyses 08, 09, and 10 comprised Exp2. Pearson's linear correlation coefficient applied to the comparison of the experiments as well as to the influence of  $^{13}\text{C}$ -saturation on the metabolic profiles demonstrated equivalence of ITR metabolite profiling and conventional metabolite profiling (Figure 2, inset).

The average coefficient of variation was determined by using all fragment pairs which contributed to each of the comparisons. Again results of ITR metabolite profiling and conventional metabolite profiling were equivalent, however, average coefficients of correlation were smaller in ITR metabolite profiling analyses (Figure 2, inset).

Most of the labeled isotopomers from the  $^{13}\text{C}$ -saturated culture were present in amounts almost equal to the  $^{12}\text{C}$ -isotopomers from the ambient  $\delta^{13}\text{C}$ -culture. The average  $^{12}\text{C}/^{13}\text{C}$ -isotopomer ratio of all pairs from the complete MST testing set was 0.79 ( $\pm 0.40$  SD). However, some substances exhibited extreme differences, the ratios ranging between 0.01 and 2.98. These observations indicated that the process of  $^{13}\text{C}$ -saturation alone may alter the levels of metabolites. Therefore, ITR metabolite profiling analyses of multiple samples should be standardised by extracts from a single large  $^{13}\text{C}$ -saturated culture and corrected for the systematic error of  $^{13}\text{C}$ -labeling.

#### **Example 5: Preparation of a compendium of MSTs**

Compilations of MSTs from biological samples represent an approach analogous to sequencing projects of expressed sequence tags (EST). We characterised the relevant major metabolites of yeast samples, obtained mass spectra and retention time indices for reliable metabolite identification, and finally generated means for metabolite-specific relative quantification.

Recently introduced GC-TOF-MS technology (van Deursen, 2000; Wagner, 2003) was adapted to the metabolic profiling of yeast. Fast scanning GC-TOF-MS systems are ideally suited for metabolite compendium projects. These systems allow automated and comprehensive deconvolution of mass spectral components from highly complex samples without user intervention. Moreover, this novel technology combines the advantages of high chromatographic resolution and reproducibility with the equally high reproducibility and acquisition rate of non-scanning time-of-flight MS-technology. In vivo stable isotope labeling was used to facilitate one of the most time-consuming steps in establishing metabolite profiling of any given biological sample type, i.e. the task to differentiate between MSTs which originate from yeast metabolism and MSTs which represent experimental contaminations. The stable isotope label was introduced as a chemically defined and predominant carbon source and was used to detect all metabolic conversions originating from this carbon source. The apparent complexity of initial metabolic profiles of polar extracts from yeast was lower than profiles generated for instance from plant sources. We increased the final

efficiency of multi-parallel GC-TOF-MS analyses by adapting metabolic profiling to combined chloroform and methanol extracts from yeast which contained lipid metabolites in addition to the metabolites obtained by polar extraction as described earlier. Further attempts to increase the amount of yeast extract to be applied to GC-TOF-MS analyses in order to maximise the number of simultaneously monitored compounds were limited by matrix effects, which were brought about by four predominant compounds, phosphoric acid (3TMS), glycerol (3TMS), glucose (MX, 5TMS), and trehalose (8TMS). The matrix effects resulted (1) from excess phosphoric acid within extracts, which reduced the silylation strength of the MSTFA reagent and (2) from chromatographic overload of derivatives which produced peak deformation artefacts in the vicinity of major peaks. The final amount of yeast extract was adjusted to avoid these matrix effects (Figure 3). Thus the efficiency of multi-parallel GC-TOF-MS analyses was increased, for the time being without introducing time-consuming pre-fractionation and enrichment protocols.

A compendium of GC-TOF-MS metabolite tags was separately compiled from ambient  $\delta^{13}\text{C}$ - and  $^{13}\text{C}$ -saturated yeast extracts from over-night batch cultures of *Saccharomyces cerevisiae* strain BY4741. In order to obtain different samples the metabolite profiles of which can be compared, different sampling protocols were applied, namely quenching into cold methanol (MEOH), collection onto filter disc (FILTER), collection by centrifugation without media wash (SPIN), and collection by repeated wash and centrifugation cycles (SPINW). The initial set of automatically retrieved mass spectra was manually curated to select MSTs of metabolic origin. The criteria applied for curation were: repeated occurrence of the mass spectral component ( $n > 3$ ), reproducible fragment composition, signal to noise  $\geq 50$ , and presence of a co-eluting  $^{13}\text{C}$ -isotopomer. Mass spectra of metabolite derivatives devoid of carbon, and metabolite derivatives originating from ambient  $\delta^{13}\text{C}$  auxotrophic and vitamin supplementation were included. The MST compendium is depicted in Table 3.

#### **Example 6: Identification and classification of MSTs**

For the identification of MSTs, mass spectral matching algorithms were employed, which are contained in publicly available mass spectral search and comparison software (Stein, 1999; Ausloos, 1999). The underlying procedures are analogous to those employed in BLAST analyses of ESTs. MSTs were compared to commercial MS collections and a custom EI-TOF-MS library. Best matches were assigned for a preliminary identification (Table 3). However, the presence of multiple chemical isomers with close to identical mass spectral fragmentation patterns make it necessary to conduct standard addition experiments in order to obtain a precise identification. We sampled 180 MSTs (Table 3) and identified 78 tags which represented 67 yeast metabolites (Table 1). The range of identified compounds comprised amino acids, organic acids, sugars, polyols, purines and pyrimidines, phosphorylated compounds, fatty acids and sterols (Table 1).

A non-biased, automated classification of MSTs has previously been established (Wagner, 2003). This approach towards a non-biased mass spectral classification utilises the observation that two mass spectra of the same compound do not only match best but also have similar match values when compared to other, even highly different, mass spectra. This method of MST classification was applied to yeast MSTs and a framework of known mass spectra obtained from standard addition experiments. We inferred 19 groups of MSTs from agglomerative hierarchical clustering by average linkage of Euclidian distances and a cut-off at approximately 50 % diversity (Figure 4 and Table 5). The groups of MSTs comprised alkanes which were included for RI standardisation (group 1; 0/7 non-identified), di- and tri saccharides (group 2; 4/17 non-identified), hexose pyranosides (group 3; 8/9 non-identified), hexonic acids and inositol (group 4; 4/10 non-identified), aldohexose methoxyamines (group 5; 3/12 non-identified), a group of non-identified MSTs similar to polyols (group 6; 5/5 non-identified), ketohexose- and pentose methoxyamines (group 7; 0/14 non-identified), hexitols, pentitols and hexonolactones (group 8; 2/19 non-identified), a group of standard caffeoylquinic acids (group 9; 0/8 non-identified), organic acids and purine nucleosides (group 10; 8/34 non-identified), C3-C5 polyols, hydroxy acids and sugars (group 11; 9/30 non-identified), phosphates (group 12; 9/34 non-identified), amines and amino acids with primary amino-group (group 14; 8/26 non-identified), fatty acids and sterols (group 15; 7/15 non-identified), a standard set of phenylpropanoic acids (group 16; 0/9 non-identified), a heterogenous group of

mostly cyclic compounds comprising phenyl-, indoyl-, imidazol-, pyrimidine-, and purine-residues (group 17; 12/31 non-identified), and a group dominated by amino acids (group 18; 9/60 non-identified). Group 0 (17 MSTs) and group 3 (4 MSTs) represented mass spectra with unclear classification. Most of those mass spectra, which represented identical compounds were found to be either nearest neighbours or were classified to belong to the same branches of the clustering tree. The mass spectrum of leucine (2TMS) was entered in duplicate in order to monitor the position of a pair of identical mass spectra within the clustering tree (Figure 4). Some yeast MSTs of group 0, namely methionine (2TMS), adenine (2TMS), and proline (2TMS), did not sort as expected. This observation was caused by errors of automated deconvolution due to low abundance or due to co-elution of other MSTs. Clustering after substitution of the matrix by a minimum threshold match value allowed improved grouping of missorted mass spectra, but obscured classification of those MSTs without high similarity to other MSTs or standard MS. More elaborate, preferably supervised-learning algorithms applied to matrices of match values as well as directly to mass spectra and RI will lead to improved and more precise classification results and increased robustness of identification.

#### **Example 7: Application of metabolite profiling analyses**

Metabolites are embedded within a network of fast enzyme and transport reactions. Not unexpectedly, metabolite co-response was discovered within sets of GC-MS metabolite profiles from plant samples. This co-response was subsequently discussed to yield novel information about biochemical mechanisms of metabolite interactions. Because reaction rates of metabolic conversions are in general significantly higher than rates of protein or mRNA turn-over, this type of analyses highly depends on a quick quenching of the metabolism during sample preparation. However, shock-freezing in liquid nitrogen, which was described earlier to be successful for plant samples, cannot be applied to yeast liquid cultures. For this reason, four other sampling regimes were assessed. These were applied to aliquots from a single batch culture. The sampling strategies were as described above (see Example 5), namely MEOH-, FILTER-, SPIN-, and SPINW-sampling by two repeated wash and centrifugation cycles of SD medium without carbohydrate source. The

metabolic perturbation induced by the respective sampling technologies was monitored by GC-TOF-MS metabolite profiles.

Principal component analyses (PCA) of all GC-TOF-MS metabolite profiles demonstrated that each of the sampling strategies exhibited specific metabolic characteristics (Figure 5). Sampling by repeated wash and centrifugation cycles (SPINW) with glucose-free SD medium was distinct from SPIN sampling and other sampling methods as described by principal component 1, which comprised the bulk variance, 57.4 %, of this experiment. Component 2, which held 24.2 % of total variance, separated sampling by centrifugation, i.e. SPIN and SPINW, from other sampling technologies. Component 3 comprising 6.4 % of total variance still allowed separation of MEOH from FILTER samples. All subsequent principal components were of low descriptive value with respect to the effect of the four sampling technologies. Analyses of the first three component loadings showed that lysine, asparagine, leucine, homoserine, methionine, arabinose, glycerol, octadecanoic acid, and 15 non-identified MSTs contributed most to the variance introduced by the choice of experimental perturbation (Table 6).

All sampling methods tested had a similar range of reproducibility as was indicated by the average relative standard deviation (RSD) of all replicate metabolite measurements (Figure 5). However, reproducibility of metabolite measurements were in some cases much lower than observed in plant samples. For example, the most widely accepted method, i.e. sampling of yeast cultures into cold methanol (MEOH), exhibited high variation for aspartic and glutamic acid, 67.2 % and 91.6 % RSD, respectively. This high variance was not caused by a trend over time of sampling or GC-TOF-MS analyses. In contrast, we demonstrated that other sampling strategies allowed highly reproducible measurements of these compounds, as was indicated for example by 18.0 % RSD with aspartic acid after FILTER sampling and 7.0 % RSD with glutamic acid after SPINW sampling. A complete overview of detailed metabolite-specific data is given in Table 6.

The data provided herein point toward the conclusion that some metabolite pools were in fast transition during or in between MEOH sampling. With respect to some metabolites, for example aspartic acid (Figure 7A) and glutamic acid, fast SPIN sampling was highly similar to MEOH sampling in exhibiting rapidly changing



metabolite pools. Finally, slower sampling technologies, like FILTER and SPINW, apparently allowed adjustment of stable metabolite pools prior to sampling.

### **Example 8: Metabolite co-response analyses**

The analyses presented in Example 7 appear to reflect rapidly changing pool sizes of some metabolites. Thus, the metabolic perturbations, which were caused by the sampling procedures, were employed in order to gain insight into metabolite/metabolite interactions. Four co-response measures, namely Pearson's correlation coefficient, Kendall's correlation coefficient, mutual information (Steuer, 2002), and Euclidian distance, were applied to characterise all pair wise metabolite combinations. The results of these analyses are shown in Table 7.

Pearson's correlation coefficient and Kendall's correlation coefficient were applied to screen for linear co-response, which was reported to prevail in similar analyses of plants. The combination of both parametric and non-parametric tests allowed a preliminary evaluation of the import of outlying measurements on each metabolite co-response. Only a small fraction of apparent linear metabolite co-responses were caused by outlying metabolite measurements (Figure 6C). When comparing Kendall's and Pearson's correlation coefficients, which were applied to the same metabolite pairs, we observed a roughly sigmoidal relationship with positive and negative linear correlation distributed almost equally. A typical example of a negative linear co-response referring to the metabolite pair glycine/uracil is shown in Figure 6C.

Mutual information of metabolite pairs plotted over Kendall's correlation coefficient shows a minimum at Kendall's correlation coefficient close to zero. The mutual information measure confirmed positive and negative linear co-response. Moreover, selecting metabolite pairs with high mutual information and low Kendall's correlation coefficient allowed to discriminate non-linear or, as shown for glycine and alanine (Figure 6B), conditionally linear metabolite co-response.

Euclidian distance proved to be a measure apparently independent of linear correlation (Figure 6A) or mutual information (data not shown). Euclidian distance, however, was highly efficient in selecting metabolite co-responses which exhibited low variance of both metabolites.

Because each of the correlation measures had different properties, it was refrained in the present work from global hypothesis-free metabolite classification through cluster analyses based on any single distance measure. Instead by selecting intermediates and products of the tricarboxylic acid cycle, we posed the question as to whether the metabolites of a common pathway may be correlated. Succinic acid, fumaric acid, malic acid, aspartic acid, and citric acid were covered by the GC-TOF-MS analyses of yeast cultures presented herein. Aconitic acid, isocitric acid, and 2-oxoglutaric acid can be analysed by GC-TOF-MS profiling but were below limits of detection in this experiment. In a first approach, we focused on those metabolite co-responses which refer to direct links by biochemical reactions (Figure 7). Highly linear correlations were observed for succinic acid, fumaric acid and malic acid, which were maintained throughout all types of sampling (Figures 7C and 7D). By contrast, malic acid and citric acid or aspartic acid, respectively, adopted seemingly independent sampling specific states (Figures 7A and 7B). These states were either linear (Figures 7A and 7B; FILTER subset) or of highly variable and non-linear nature. Other metabolites, which are known to be directly interlinked by biochemical reactions, were also found to be correlated, for example lanosta-8,24-dien-3-beta-ol and ergosterol, glucose-6-phosphate and fructose-6-phosphate, or hexadecanoic acid and octadecanoic acid (Table 7).

In addition, interactions which did not follow classical pathway definitions were found within the data set of metabolite co-responses. For example, we selected a group of corresponding metabolites from a biochemical path of interest, namely succinic acid, fumaric acid, and malic acid, and searched for common closest neighbours. The 3 closest neighbours of this group of organic acids were glyceric acid and two non-identified metabolites as judged by positive Kendall's correlation coefficient. In addition lysine, glycine, and glutamic acid were most distant as judged by negative Kendall's correlation coefficient. An overview of this analyses is shown as a network representation (Figure 8).

#### **Example 9: $^{13}\text{C}$ -ITR metabolite profiling by MALDI-TOF mass spectrometry**

Metabolite profiling by GC-TOF-MS was shown to cover about 11% of the 584 yeast metabolites which were predicted by genome-scale reconstruction (Forster, 2003). However, this approach is mainly restricted by the limited scope of the GC-TOF-MS technology. The focus on specific classes of compounds with common properties is inherent to this as well as to any other analytical technology. For this reason, it is demonstrated in connection with the present invention that metabolite profiling using  $^{13}\text{C}$ -in vivo labeling can be extended to MALDI-TOF-MS. MALDI-TOF-MS represents a mass spectral technology, which (1) cannot rely on chromatography for the confirmation of substance identity, (2) is highly sensitive to matrix suppression effects during laser desorption and ionisation, and (3) is not suited for external quantitative calibration. However, using MALDI-TOF for quantification with internal standard substances which are labeled by stable isotopes is an accepted procedure in connection with metabolite flux analyses (Wittmann, 2002; Wittmann, 2001). By nicotinamide adenine dinucleotide (NADH;  $\text{C}_{21}\text{H}_{29}\text{N}_7\text{O}_{14}\text{P}_2$ ), an ubiquitous metabolic co-factor was chosen which allowed the demonstration of prerequisites essential to the  $^{13}\text{C}$ -ITR approach.

Yeast extracts were treated as described above (see Example 4) to yield samples of a third experiment (Exp3). These samples were each harvested from the same batch cultures. Extracts with ambient  $\delta^{13}\text{C}$  composition, extracts with  $^{13}\text{C}$ -saturated metabolites, and an equal mixture of both extracts were analysed. Screening of MALDI-TOF spectra from the ambient  $\delta^{13}\text{C}$  extract revealed protonated molecular ions of  $\text{NAD}^+$  and NADH at  $m/z$  664.11 and  $m/z$  666.13, as well as sodium adducts at  $m/z$  686.09 and 688.12 (Figure 9). These identifications were supported by commercial preparations of  $\text{NAD}^+$  and NADH. The mass resolution of the MALDI-TOF system did not allow separation of the mono-isotopic  $^{12}\text{C}$ -NADH ion from the A+2 isotopomer of ambient  $\text{NAD}^+$ . Therefore, analogous to the quantification of glycine (3TMS) (Figure 1), correction will be required for the determination of NADH in the presence of  $\text{NAD}^+$ . In addition, MALDI-TOF generated a continuous evenly spaced background of signals (Figure 9).

Within the mixed sample (Figure 9, inset), we found isotopomers of the protonated molecular ions of  $\text{NAD}^+$  and NADH, which contained 15  $^{13}\text{C}$ -atoms out of 21 carbon atoms present within NAD(H). Small amounts of labeled sodium adducts were present (data not shown). The presence of only 15 labeled carbon atoms was in

agreement with the incorporation of non-labeled nicotinamide moieties into NAD(H), which originated from the nicotinic acid vitamin supplement contained in the yeast SD medium. The presence of non-labeled nicotinic acid ( $C_6H_5NO_2$ ) in  $^{13}C$ -labeled yeast extracts was demonstrated above (Example 1).

The identification of NAD(H) within yeast extracts was confirmed by post source decay (PSD) fingerprints of the protonated molecular ion cluster which were recorded separately from the ambient  $\delta^{13}C$  and the  $^{13}C$ -saturated yeast extracts (Figure 10). Analogous to the comparison of GC-EI-MS fragmentation pattern of isotopomers (Figure 1), head-to-tail analyses of PSD fingerprints allows the verification of the correct choice of isotopomer pairs. Moreover, fragment analyses of the  $^{12}C$ -PSD and the  $^{13}C$ -PSD revealed the successive loss of three moieties containing 5 carbon atoms each, namely two ribose units and one adenine building block, as was indicated by mass differences of 5, 10, and 15, respectively. Due to the restricted resolution of PSD analyses, separate fingerprints of the protonated ions of  $NAD^+$  and NADH could not be obtained from mixtures. However, commercially available preparations of  $NAD^+$  and NADH indicated that some PSD fragments, for example the fragment  $m/z$  649.4  $[M-17]^+$ , were highly specific. Fragment  $m/z$  649.4 may result from facilitated neutral loss of  $NH_3$  from the protonated NADH molecular ion. MALDI-TOF preparations of commercially available  $NAD^+$  exhibited variable amounts of NADH mainly in the form of ion  $m/z$  666.13, whereas  $NAD^+$  was not detectable in preparations from NADH. This last finding indicated that the chosen MALDI-TOF procedure generates a reducing environment for chemical analyses which requires monitoring.

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**Table 1**

Table of yeast metabolites, which were represented by at least one mass spectral tag (MST). Identification of MSTs was performed by standard addition experiments. Identification required co-elution, mass spectral similarity, and presence of differentially labeled isotopomers.

**Amino acids**

2-Aminoadipic acid  
Alanine  
Arginine  
Asparagine  
Aspartic acid  
Cysteine  
Glutamic acid  
Glutamine  
Glycine  
Histidine  
Homocysteine  
Homoserine  
Isoleucine  
Leucine  
Lysine  
Methionine  
Ornithine  
Phenylalanine  
Proline  
Pyroglutamic acid  
Serine  
Threonine  
Tryptophan  
Tyrosine  
Valine

**Organic acids**

Citramalic acid  
Citric acid  
Erythronic acid  
Fumaric acid  
Gluconic acid  
Glyceric acid  
Malic acid  
Pantothenic acid  
Succinic acid

**Miscellaneous**

Adenine  
Ethanolamine  
Nicotinic acid  
Uracil  
Urea

**Fatty acids**

9-(Z)-Octadecenoic acid  
Hexadecanoic acid  
Octadecanoic acid  
Octadecenoic acid

**Sterols**

Ergosterol  
Lanosta-8,24-dien-3-beta-ol

**Sugars**

alpha-D-Methylglucopyranoside  
Arabinose  
Ribose  
Fructose  
Fucose  
Glucose  
Isomaltose  
Mannose  
Trehalose

**Polyols**

Erythritol  
Glycerol  
myo-Inositol  
Mannitol  
Ribitol  
Sorbitol

**Phosphates**

Fructose-6-phosphate  
Glucose-6-phosphate  
Galactose-6-phosphate  
Glyceric acid-3-phosphate  
Glycerol-2-phosphate  
Glycerol-3-phosphate  
Phosphoric acid

**Table 2**

The table includes all manually evaluated GC-EI-MS isotopomer fragment pairs of identified and non-identified metabolite derivatives used for  $^{13}\text{C}$ -ITR metabolite profiling. The table comprises names of metabolite derivatives or of best matches, mass spectrum identifier (MS-ID) for cross-referencing with Table 3, mass to charge ratio (M/Z) characterising the fragment isotopomer pairs and deviation of retention time indices ( $\Delta\text{RI}$ ).

**Table 3**

Datafile in the format \*.msp<sup>a</sup> containing all curated GC-EI-TOF-MS mass spectra of MSTs from extracts of *Saccharomyces cerevisiae* strain BY4741.

The spectrum name was designed to allow sorting according to isotopomer, retention time index, experiment, and name, for example 12C\_1625.9\_1274EC17\_Glutamic acid (3TMS) or 12C\_1802.0\_1313EC75\_[706; Xylitol (5TMS)]. Retention time indices are as observed within the indicated experiment. Names represent identifications by co-elution and mass spectral match<sup>b</sup>; names in brackets indicate non-identified compounds and include the best mass spectral match. The chemical ID field was used to group isotopomer mass spectra by a common mass spectral ID (MS-ID), for example 163001-10-1 and 163001-11-1 representing ambient  $\delta^{13}\text{C}$ - and  $^{13}\text{C}$ -saturated isotopomers of glutamic acid (3TMS). This identifier does not represent a CAS registry number. The formatting of this field is predefined by AMDIS software.

<sup>a</sup> The file format \*.msp can be imported into NIST98 and NIST02 mass spectral comparison software (to be downloaded from [http://chemdata.nist.gov/mass-spc/Srch\\_v1.7/index.html](http://chemdata.nist.gov/mass-spc/Srch_v1.7/index.html) or AMDIS software (to be downloaded from <http://chemdata.nist.gov/mass-spc/amdis/>).

<sup>b</sup> By-products observed in preparations of reference substances were marked (BP).

**Table 4**

Matrix of all mass spectral similarities of the MSTs from yeast which are presented in Table 3. A complete pair-wise matching was performed with NIST98 mass spectral search and comparison software.

**Table 5**

Table of identified and non-identified MSTs from extracts of *Saccharomyces cerevisiae* strain BY4741 and pure standard compounds. MSTs were classified into groups by hierarchical clustering of the complete symmetric matrix of pair-wise mass spectral match values (Table 4). The resulting clustering tree is shown in Figure 4.

**Table 6**

Table of metabolite responses from GC-TOF-MS metabolite profiles of four sampling strategies ( $n = 6$ ), namely MEOH-, FILTER-, SPIN- and SPINW-sampling by two repeated wash and centrifugation cycles. All samplings were performed on a single batch culture of *Saccharomyces cerevisiae* strain BY4741 ( $A_{595} \sim 1.8$ ). Metabolite responses were normalised by the average metabolite response observed within each sample. MSTs and fragments which comprised the metabolite responses in this set of experiments are indicated. Metabolites exhibiting more than 75% missing data in all types of sampling strategies were removed. Table 6A depicts the raw data values which gave rise to the average values depicted in Table 6B.

**Table 7**

Table of all pair-wise metabolite/metabolite co-response measures. Number of available pair-wise measurements, Euclidian distance, mutual information, Kendall's- and Pearson's correlation coefficient were calculated from the metabolite responses presented in Table 6. The global information content of the correlation measures is demonstrated in Figure 6.

**Table 2**

<b>DERIVATIVE [BEST MATCH; NAME]</b>	<b>MS-ID</b>	<b>ISOTOPOMER PAIR M/Z</b>	<b><math>\Delta</math> RI</b>
Alanine (2TMS)	110001	116_118 190_192 218_221	0.00 0.00 0.18
Glycine (3TMS)	133001	174_175 248_249 276_278	0.00 0.00 0.36
Threonine (2TMS)	132001	117_119 219_221 130_133	0.57 0.93 -0.75
Alanine (3TMS)	138002	188_190 100_102 262_264	0.00 0.00 0.18
Serine (3TMS)	138001	204_206	0.30
Aspartic acid (3TMS)	152002	232_235 292_294 306_309	0.00 0.00 0.25
Pyroglutamic acid (2TMS)	153002	156_160 230_234 258_263	0.00 0.23 0.23
Glutamic acid (3TMS)	163001	246_250 128_131 230_234	0.23 0.00 0.23
Phenylalanine (2TMS)	164001	218_220 192_200 266_274	0.45 0.45 0.23
Asparagine (3TMS)	168001	116_118	0.00
Ornithine (3TMS)	176006	174_175 348_353	0.23 0.00
Ornithine (4TMS)	182002	142_146 174_175 420_425	0.00 0.23 0.00
Arginine (5TMS)	183001	157_161 256_261 373_379	0.25 0.20 0.43
Tyrosine (2TMS)	189006	179_186 91_98	0.25 0.71

Lysine (4TMS)	192003	156_161	1.67
		174_175	0.00
		317_322	0.27
Lysine (3TMS)	186002	174_175	0.00
		200_206	0.00
		258_264	0.00
Tyrosine (3TMS)	194002	218_220	0.58
		280_288	0.00
		354_362	0.00
Glycerol (3TMS)	129003	218_221	0.00
		263_265	0.20
		293_296	0.00
Fructose methoxyamine (5TMS)	187002	217_220	0.23
		307_310	0.45
Fructose methoxyamine {BP} (5TMS)	188004	307_310	0.96
		217_220	0.00
Mannose methoxyamine (5TMS)	188002	205_207	0.23
		217_220	0.00
		319_323	0.23
Glucose methoxyamine (5TMS)	189002	364_368	-0.06
		343_349	0.24
		291_294	0.00
Glucose methoxyamine {BP} (5TMS)	191001	364_368	1.12
		343_349	1.97
		291_294	1.39
Mannitol (6TMS)	193002	217_220	1.06
		319_323	0.00
Sorbitol (6TMS)	193001	217_220	0.00
		319_323	0.00
Trehalose (8TMS); alpha-D-Glc-(1,1)-alpha-D-Glc	274002	451_457	3.32
		243_248	3.28
		435_441	3.32
Succinic acid (2TMS)	134001	247_251	0.18
		172_176	0.55
		248_252	0.67
Citramalic acid (3TMS)	148001	115_118	0.39
		247_251	0.39
		259_264	0.20
Malic acid (3TMS)	149001	233_236	0.00
		245_249	0.39
		335_339	0.18
Citric acid (4TMS)	182004	273_278	0.23

		347_352	0.23
		465_471	0.23
Glycerol-3-phosphate (4TMS)	177002	445_448	0.10
Fructose-6-phosphate methoxyamine (6TMS)	232002	217_220	0.00
		459_462	0.00
Glucose-6-phosphate methoxyamine (6TMS)	233002	471_475	-0.32
		160_162	0.32
[644; 2-Methyl-1,3-butanediol (2TMS)]	140003	117_119	0.00
		306_309	0.36
[700; 2-methyl-1,2-propanediol (2TMS)]	141003	131_134	0.00
		292_294	0.00
		277_279	0.36
[725; 2-Ketooctanoic acid (2TMS)]	146003	185_191	0.18
		212_219	0.36
		287_294	0.18
[545; 2,3-Dimethylsuccinic acid (2TMS)]	149003	291_298	0.18
		275_281	0.18
		207_209	0.18
[815; Ethyl-3(2H)-thiophenone]	150003	128_131	0.14
[729; N,N-Dimethyllysine methyl ester]	151003	128_131	0.71
		84_88	0.00
[680; 2,3-Dimethylsuccinic acid (2TMS)]	158003	287_294	0.45
		377_384	0.23
[882; Ornithine (3TMS)]	162001	142_146	0.00
		348_353	0.43
		115_117	0.00
[548; Leucine (2TBS)]	165002	315_320	0.00
		200_203	0.00
		330_335	-0.25
[612; 4-Aminobutyric acid (2TBS)]	175003	112_118	0.23
		274_280	0.25
		376_383	0.58
[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	176005	184_189	0.23
[829; Orotic acid (3TMS)]	176003	254_258	0.25
		357_362	0.00
		269_274	-0.23
[757; 2-Desoxy-pentos-3-ylose dimethoxyamine (2TMS)]	176004	231_235	0.00
		315_321	0.61
[812; D-Xylofuranose (4TMS)]	177004	305_308	-0.15
[731; Erythrose (3TMS)]	184003	117_119	0.23

		217_220	0.23
		204_206	0.45
[826; beta-[[[(5-methyl-2-thienyl)methylene]amino]-benzeneacetic acid methyl ester]	187004	241_245	0.20
		431_437	0.00
		153_157	0.23
[772; D-Glucose (5TMS)]	189005	204_206	0.10
[793; D-Galactono-1,4-lactone (4TMS)]	196004	217_220	0.00
		243_248	0.00
		361_367	0.55
[945; beta-D-Glucopyranose (5TMS)]	197002	191_192	0.00
		204_206	0.00
		217_220	0.00
[775; Dopamine (4TMS)]	200002	174_175	0.00
		317_324	0.55
		375_382	0.55
[680; Glycerol-2-phosphate (4TMS)]	203004	243_248	0.58
		258_263	0.58
		169_174	0.85
[766; beta-D-Methylglucopyranoside (4TMS)]	203003	204_206	0.00
		259_264	0.00
		319_323	0.00
[607; Putrescine (4TMS)]	204003	375_379	-0.18
[756; beta-D-Methylglucopyranoside (4TMS)]	209004	204_206	0.27
		319_323	0.27
		243_248	0.55
[662; Ribose-5-phosphate methoxyamine {BP} (5TMS)]	211004	299_299	0.00
		315_315	0.00
[648; Ethylamine (2TMS)]	216002	174_175	0.00
		217_220	0.00
		345_349	-0.27
[705; 2-Ketogluconic acid (5TMS)]	217002	437_442	0.00
		257_262	0.00
		217_220	0.27
[733; Threitol (4TMS)]	218001	217_220	0.27
[715; Erythritol (4TMS)]	226001	373_382	0.46
		217_220	0.32
[945; Uridine (3TMS)]	248002	217_220	0.32
		259_264	0.32
[644; Erythritol (4TMS)]	252002	446_454	0.64
		217_220	0.00



[895; Isomaltose methoxyamine (8TMS)]	281001	204_206	0.32
		361_367	0.32
[542; Maltose methoxyamine {BP} (8TMS)]	282003	204_206	0.80

Table 3

NAME:13C\_1731.2\_1313EC11\_Ribitol (5TMS)  
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
 CASNO:173001-11-1

RI:1731

RT:10.550

NUM PEAKS: 41

( 70	3)	( 72	18)	( 73	1000)	( 74	80)	( 75	63)
( 87	8)	( 89	7)	( 90	22)	(103	32)	(104	189)
(105	13)	(106	5)	(119	83)	(131	28)	(132	120)
(133	70)	(134	12)	(146	11)	(147	318)	(148	50)
(149	30)	(191	50)	(192	20)	(206	53)	(207	98)
(208	18)	(209	6)	(220	215)	(221	71)	(222	20)
(223	4)	(248	15)	(279	9)	(280	4)	(281	4)
(310	23)	(311	6)	(322	8)	(323	42)	(324	12)
(325	5)								

NAME:13C\_1318.4\_1313EC16\_Proline (2TMS)  
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
 CASNO:132003-11-1

RI:1318

RT:6.620

NUM PEAKS: 19

( 70	7)	( 71	17)	( 72	28)	( 73	600)	( 74	60)
( 80	7)	( 84	5)	( 85	17)	( 86	5)	(115	6)
(128	4)	(142	4)	(143	3)	(144	20)	(145	39)
(146	1000)	(147	90)	(148	33)	(220	38)		

NAME:13C\_1318.9\_1313EC16\_Threonine (2TMS)  
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
 CASNO:132001-11-1

RI:1319

RT:6.627

NUM PEAKS: 58

( 73	1000)	( 75	547)	( 76	49)	( 77	23)	( 79	8)
( 81	58)	( 82	5)	( 88	115)	( 89	29)	( 90	4)
( 91	3)	( 92	3)	( 93	7)	( 96	4)	(102	45)
(103	54)	(104	22)	(105	15)	(106	4)	(114	3)
(116	11)	(117	80)	(118	56)	(119	667)	(120	55)
(121	21)	(129	2)	(130	7)	(132	40)	(133	663)
(134	170)	(135	38)	(136	6)	(149	335)	(150	30)
(151	12)	(153	3)	(159	5)	(161	7)	(162	31)
(178	4)	(190	2)	(191	2)	(192	2)	(205	7)
(206	17)	(207	10)	(208	3)	(210	2)	(221	193)
(222	33)	(223	27)	(224	5)	(225	3)	(234	5)
(235	3)	(252	18)	(253	3)				

NAME:13C\_1413.9\_1313EC16\_  
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
 CASNO:141004-11-1

RI:1414

RT:7.745

NUM PEAKS: 27

( 72	44)	( 73	604)	( 74	142)	( 75	1000)	( 76	120)
( 77	113)	( 87	85)	( 88	70)	(103	47)	(104	71)
(105	62)	(106	26)	(117	85)	(118	29)	(119	145)
(120	39)	(121	447)	(132	323)	(133	198)	(148	76)
(151	59)	(160	25)	(161	22)	(162	190)	(163	21)
(164	15)	(177	23)						

NAME:13C\_1420.9\_1313EC16\_Alanine {BP} (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:142001-11-1

RI:1421

RT:7.827

NUM PEAKS: 34

( 72	122)	( 73	1000)	( 74	112)	( 75	354)	( 76	29)
( 87	18)	( 88	23)	(100	78)	(101	25)	(102	73)
(103	27)	(104	12)	(115	7)	(117	42)	(118	517)
(119	48)	(120	17)	(131	20)	(133	52)	(134	8)
(146	38)	(147	353)	(148	56)	(149	49)	(162	420)
(163	42)	(164	15)	(190	15)	(192	115)	(193	20)
(236	20)	(265	75)	(266	15)	(267	6)		

NAME:13C\_1489.8\_1313EC16\_Malic acid (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:149001-11-1

RI:1490

RT:8.637

NUM PEAKS: 59

( 70	3)	( 72	30)	( 73	1000)	( 74	90)	( 75	140)
( 76	9)	( 87	10)	(101	31)	(102	8)	(103	53)
(104	6)	(105	6)	(115	10)	(117	23)	(118	23)
(119	9)	(131	30)	(132	11)	(133	127)	(134	17)
(135	12)	(143	7)	(146	10)	(147	413)	(148	62)
(149	46)	(150	5)	(151	9)	(175	29)	(176	9)
(177	30)	(178	12)	(189	19)	(190	16)	(191	60)
(192	20)	(193	6)	(206	5)	(207	4)	(217	8)
(220	12)	(221	11)	(234	7)	(235	6)	(236	46)
(237	8)	(245	18)	(249	27)	(250	6)	(251	4)
(263	4)	(265	13)	(266	11)	(308	5)	(309	4)
(310	9)	(319	3)	(323	4)	(339	9)		

NAME:13C\_1495.3\_1313EC16\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:150003-11-1

RI:1495

RT:8.703

NUM PEAKS: 52

( 72	21)	( 73	574)	( 74	66)	( 75	184)	( 76	15)
( 77	11)	( 86	8)	( 87	17)	( 88	7)	( 89	6)
( 95	3)	(100	5)	(101	37)	(102	45)	(103	20)
(104	15)	(105	7)	(115	11)	(116	6)	(117	26)
(118	9)	(119	37)	(120	3)	(121	3)	(129	6)
(130	47)	(131	1000)	(132	133)	(133	81)	(134	10)
(135	3)	(146	3)	(147	74)	(148	12)	(149	14)
(160	9)	(161	5)	(162	11)	(176	4)	(177	6)
(193	96)	(194	8)	(195	3)	(204	16)	(205	51)
(206	12)	(207	4)	(220	9)	(221	3)	(234	12)
(296	4)	(311	3)						

NAME:13C\_1521.6\_1313EC16\_Aspartic acid (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:152002-11-1

RI:1522

RT:8.925

NUM PEAKS: 74

( 70	7)	( 71	9)	( 72	28)	( 73	1000)	( 74	104)
( 75	156)	( 76	11)	( 77	8)	( 84	3)	( 85	6)
( 86	7)	( 87	13)	( 88	4)	( 89	5)	(100	13)
(101	93)	(102	157)	(103	26)	(104	15)	(105	4)

(115	6)	(116	7)	(117	17)	(118	23)	(119	40)
(120	4)	(121	5)	(130	5)	(131	28)	(132	42)
(133	52)	(134	11)	(135	7)	(145	17)	(146	10)
(147	157)	(148	28)	(149	26)	(150	4)	(162	3)
(163	21)	(164	4)	(173	3)	(174	7)	(175	11)
(176	9)	(178	5)	(189	3)	(190	44)	(191	11)
(192	5)	(203	3)	(204	40)	(205	11)	(206	13)
(207	4)	(218	4)	(219	21)	(220	71)	(221	18)
(222	7)	(233	4)	(234	20)	(235	357)	(236	64)
(237	30)	(238	4)	(248	4)	(249	3)	(294	5)
(309	10)	(310	3)	(338	5)	(353	3)		

NAME:13C\_1594.8\_1313EC16\_  
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
 CASNO:159001-11-1  
 RI:1595  
 RT:9.493

NUM PEAKS: 33

( 70	10)	( 72	58)	( 73	1000)	( 74	105)	( 75	173)
( 86	10)	( 87	21)	(100	20)	(101	51)	(102	30)
(115	14)	(117	40)	(118	15)	(131	20)	(133	37)
(139	12)	(144	17)	(145	36)	(146	575)	(147	211)
(148	48)	(174	9)	(175	15)	(189	15)	(190	388)
(191	40)	(192	14)	(220	128)	(221	21)	(222	9)
(293	36)	(294	8)	(295	4)				

NAME:13C\_1630.8\_1313EC16\_Glutamic acid (3TMS)  
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
 CASNO:163001-11-1  
 RI:1631  
 RT:9.772

NUM PEAKS: 83

( 70	7)	( 71	9)	( 72	28)	( 73	1000)	( 74	99)
( 75	255)	( 76	18)	( 85	9)	( 86	13)	( 87	29)
( 88	162)	( 89	11)	( 99	4)	(100	11)	(101	62)
(102	61)	(103	20)	(104	14)	(105	5)	(113	3)
(114	3)	(115	30)	(116	11)	(117	43)	(118	20)
(119	11)	(129	3)	(130	15)	(131	331)	(132	76)
(133	88)	(134	16)	(135	8)	(144	33)	(145	7)
(146	8)	(147	205)	(148	38)	(149	56)	(150	8)
(151	4)	(158	5)	(159	12)	(160	164)	(161	26)
(162	38)	(163	7)	(173	4)	(174	4)	(175	5)
(176	4)	(177	3)	(178	5)	(189	3)	(190	4)
(191	6)	(205	12)	(206	29)	(207	7)	(208	3)
(218	9)	(219	6)	(220	20)	(221	22)	(222	6)
(233	5)	(234	70)	(235	16)	(236	7)	(248	5)
(249	25)	(250	438)	(251	78)	(252	36)	(253	4)
(263	9)	(279	5)	(324	6)	(352	3)	(353	30)
(355	4)	(368	15)	(369	5)				

NAME:13C\_1640.6\_1313EC16\_Phenylalanine (2TMS)  
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
 CASNO:164001-11-1  
 RI:1641  
 RT:9.848

NUM PEAKS: 69

( 70	52)	( 71	8)	( 72	19)	( 73	1000)	( 74	93)
( 75	105)	( 76	6)	( 83	12)	( 86	6)	( 87	20)
( 96	12)	( 97	17)	( 98	163)	( 99	14)	(100	5)
(101	171)	(104	9)	(110	3)	(111	13)	(112	3)

(113	3)	(117	8)	(118	5)	(119	5)	(124	3)
(125	6)	(126	10)	(127	11)	(128	12)	(132	59)
(133	33)	(134	7)	(135	3)	(138	5)	(139	8)
(140	6)	(141	6)	(145	4)	(146	4)	(147	156)
(148	30)	(149	13)	(153	3)	(154	3)	(155	3)
(159	3)	(161	4)	(163	9)	(168	13)	(169	4)
(170	5)	(175	4)	(184	9)	(185	9)	(198	3)
(199	23)	(200	267)	(201	24)	(202	8)	(205	8)
(213	10)	(219	10)	(220	377)	(221	82)	(222	33)
(223	5)	(274	23)	(275	7)	(303	6)		

NAME:13C\_1707.8\_1313EC16\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:171003-11-1

RI:1708

RT:10.369

NUM PEAKS: 168

( 70	4)	( 71	26)	( 72	27)	( 73	1000)	( 74	90)
( 75	126)	( 76	6)	( 79	3)	( 80	3)	( 85	14)
( 86	12)	( 87	22)	( 88	9)	( 89	101)	( 90	12)
( 91	8)	( 92	4)	( 93	3)	( 99	4)	(101	49)
(102	11)	(103	36)	(104	12)	(105	6)	(106	4)
(108	3)	(113	3)	(115	13)	(116	10)	(117	37)
(118	20)	(119	7)	(120	5)	(121	4)	(129	25)
(130	8)	(132	31)	(133	39)	(134	7)	(136	5)
(139	3)	(143	9)	(144	7)	(145	31)	(146	9)
(147	130)	(148	49)	(149	14)	(150	6)	(157	6)
(158	7)	(159	72)	(160	46)	(161	12)	(162	11)
(163	11)	(164	4)	(171	4)	(172	3)	(174	8)
(175	63)	(176	14)	(177	20)	(183	5)	(184	3)
(186	4)	(188	8)	(189	14)	(190	12)	(191	5)
(193	4)	(196	4)	(205	6)	(206	7)	(214	4)
(215	3)	(216	3)	(217	3)	(220	13)	(227	3)
(232	8)	(233	7)	(234	6)	(235	14)	(236	4)
(239	3)	(245	3)	(246	3)	(248	21)	(249	13)
(250	4)	(254	3)	(256	4)	(260	3)	(261	4)
(262	4)	(268	3)	(270	4)	(272	3)	(276	15)
(277	28)	(278	15)	(279	105)	(280	21)	(285	3)
(286	6)	(290	3)	(291	3)	(292	7)	(293	4)
(298	5)	(299	5)	(300	4)	(306	5)	(307	10)
(308	6)	(309	5)	(314	5)	(315	3)	(316	3)
(320	5)	(321	11)	(322	7)	(328	3)	(338	4)
(340	3)	(342	3)	(344	3)	(346	4)	(349	3)
(351	8)	(367	4)	(368	3)	(370	3)	(376	4)
(378	3)	(379	4)	(380	5)	(398	3)	(400	3)
(401	4)	(404	3)	(409	3)	(425	3)	(429	4)
(438	3)	(449	4)	(450	3)	(456	4)	(457	4)
(475	3)	(480	5)	(481	3)	(483	3)	(484	3)
(487	6)	(488	3)	(505	3)	(506	3)	(510	4)
(514	3)	(519	3)	(523	3)	(531	3)	(534	4)
(536	3)	(537	3)	(543	4)				

NAME:13C\_1720.2\_1313EC16\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:172005-11-1

RI:1720

RT:10.465

NUM PEAKS: 47

( 72	28)	( 73	767)	( 74	167)	( 75	1000)	( 76	86)
( 77	40)	( 78	9)	( 86	16)	( 87	224)	( 88	272)

( 90 186) ( 91 21) ( 92 6) (101 36) (116 9)  
(117 111) (118 155) (131 56) (133 189) (134 15)  
(135 6) (143 64) (144 35) (145 9) (146 20)  
(148 72) (149 39) (151 5) (159 269) (160 555)  
(161 142) (162 121) (163 37) (164 9) (173 7)  
(175 5) (176 53) (177 668) (178 59) (179 31)  
(205 11) (223 14) (233 71) (234 26) (235 11)  
(279 3) (280 26)

NAME:13C\_1746.9\_1313EC16\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:175003-11-1

RI:1747

RT:10.672

NUM PEAKS: 13

( 72 35) ( 73 1000) ( 74 98) ( 75 217) ( 88 144)  
( 89 106) (117 50) (118 371) (147 203) (190 40)  
(221 108) (280 293) (281 49)

NAME:13C\_1769.9\_1313EC16\_Glycerol-3-phosphate (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:177002-11-1

RI:1770

RT:10.850

NUM PEAKS: 108

( 70 5) ( 72 26) ( 73 1000) ( 74 87) ( 75 119)  
( 76 8) ( 77 18) ( 79 3) ( 90 9) ( 91 5)  
( 98 3) (102 14) (103 109) (104 98) (105 25)  
(106 5) (107 5) (115 17) (116 20) (117 11)  
(118 32) (119 25) (120 4) (121 8) (123 3)  
(131 23) (132 74) (133 123) (134 52) (135 37)  
(136 5) (137 13) (147 150) (148 24) (149 21)  
(150 3) (151 10) (153 3) (163 3) (164 5)  
(165 5) (167 4) (179 4) (181 18) (182 3)  
(183 6) (193 20) (194 4) (195 18) (196 3)  
(197 5) (205 3) (206 13) (207 39) (208 9)  
(209 6) (210 4) (211 97) (212 15) (213 9)  
(223 3) (225 20) (226 7) (227 18) (228 3)  
(242 17) (243 12) (255 8) (256 3) (257 19)  
(258 3) (269 4) (283 5) (284 3) (285 20)  
(286 5) (298 17) (299 180) (300 49) (301 25)  
(302 4) (313 3) (314 12) (315 44) (316 13)  
(317 6) (329 12) (330 4) (343 13) (344 6)  
(345 3) (358 19) (359 113) (360 34) (361 16)  
(362 3) (372 5) (373 30) (374 10) (375 5)  
(386 3) (387 12) (388 5) (389 5) (447 4)  
(448 17) (449 7) (450 3)

NAME:13C\_1771.0\_1313EC16\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:177003-11-1

RI:1771

RT:10.859

NUM PEAKS: 41

( 83 83) ( 87 766) (101 497) (111 47) (112 24)  
(129 41) (130 121) (143 46) (159 137) (160 296)  
(172 89) (173 999) (174 192) (175 1000) (176 159)  
(187 117) (188 76) (201 93) (202 342) (203 62)  
(216 111) (217 73) (248 155) (250 28) (260 38)  
(294 27) (305 25) (306 28) (333 30) (334 204)

65

(335 247) (336 98) (340 19) (350 182) (351 59)  
 (366 39) (411 26) (426 18) (514 20) (536 21)  
 (540 17)

NAME:13C\_1784.2\_1313EC16\_Glutamine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:178001-11-1

RI:1784

RT:10.961

NUM PEAKS: 88

( 70 11) ( 71 17) ( 72 32) ( 73 1000) ( 74 139)  
 ( 75 301) ( 76 22) ( 77 12) ( 84 4) ( 85 23)  
 ( 86 13) ( 87 52) ( 88 14) ( 89 7) ( 90 5)  
 ( 99 5) (100 9) (101 46) (102 33) (103 13)  
 (105 3) (113 4) (114 3) (115 28) (116 32)  
 (117 64) (118 33) (119 9) (129 13) (130 12)  
 (131 97) (132 43) (133 111) (134 15) (135 7)  
 (142 3) (143 49) (144 20) (145 11) (146 22)  
 (147 164) (148 67) (149 37) (150 6) (157 5)  
 (158 17) (159 262) (160 744) (161 87) (162 32)  
 (163 3) (172 4) (173 3) (174 6) (175 5)  
 (176 3) (177 8) (188 3) (189 6) (190 13)  
 (191 4) (203 3) (204 3) (205 67) (206 15)  
 (207 6) (217 4) (218 4) (219 9) (220 19)  
 (221 10) (231 7) (232 5) (233 27) (234 15)  
 (235 12) (248 9) (249 94) (250 17) (251 7)  
 (262 6) (263 3) (277 5) (278 7) (305 7)  
 (352 15) (353 5) (367 5)

NAME:13C\_1821.6\_1313EC16\_Ornithine (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:182002-11-1

RI:1822

RT:11.252

NUM PEAKS: 70

( 73 736) ( 74 117) ( 85 13) ( 86 15) ( 87 130)  
 ( 88 16) ( 89 6) ( 90 6) (100 18) (101 85)  
 (102 54) (103 54) (104 17) (105 3) (113 6)  
 (114 14) (115 25) (116 26) (117 41) (128 4)  
 (129 9) (130 81) (131 77) (132 32) (144 19)  
 (145 41) (146 1000) (157 8) (158 7) (159 12)  
 (160 8) (161 11) (162 4) (172 3) (173 33)  
 (174 33) (175 333) (176 61) (177 35) (178 5)  
 (189 10) (190 15) (191 11) (192 8) (202 7)  
 (203 70) (204 19) (205 20) (206 16) (218 38)  
 (219 16) (220 54) (236 3) (246 7) (247 6)  
 (248 3) (249 7) (263 28) (264 27) (265 6)  
 (290 3) (320 6) (321 4) (335 9) (336 3)  
 (410 3) (424 4) (425 23) (426 10) (427 5)

NAME:13C\_1829.5\_1313EC16\_Arginine (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:183001-11-1

RI:1830

RT:11.313

NUM PEAKS: 91

( 70 25) ( 71 20) ( 72 126) ( 73 1000) ( 74 244)  
 ( 75 99) ( 76 7) ( 84 6) ( 85 76) ( 86 27)  
 ( 87 34) ( 88 13) ( 89 11) ( 90 13) ( 98 3)  
 ( 99 11) (100 73) (101 58) (102 55) (103 16)

66

(104	14)	(113	4)	(114	6)	(115	21)	(116	14)
(117	57)	(118	14)	(123	5)	(128	13)	(129	32)
(130	22)	(131	50)	(132	36)	(133	33)	(134	6)
(142	4)	(143	18)	(144	42)	(145	105)	(146	201)
(147	110)	(148	35)	(149	10)	(156	4)	(157	9)
(158	14)	(159	46)	(160	60)	(161	521)	(162	59)
(163	20)	(171	4)	(172	35)	(173	37)	(174	16)
(177	9)	(187	3)	(188	14)	(189	9)	(190	10)
(191	5)	(192	6)	(201	3)	(202	3)	(203	3)
(204	4)	(205	3)	(217	3)	(218	3)	(219	17)
(220	29)	(221	6)	(222	3)	(234	3)	(235	5)
(245	8)	(246	4)	(248	4)	(249	18)	(250	3)
(259	4)	(260	15)	(261	189)	(262	37)	(263	16)
(264	6)	(274	4)	(289	3)	(335	3)	(364	5)
(379	7)								

NAME:13C\_1835.5\_1313EC16\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:184003-11-1

RI:1836

RT:11.359

NUM PEAKS: 91

( 71	8)	( 72	27)	( 73	1000)	( 74	86)	( 75	140)
( 76	11)	( 77	9)	( 86	13)	( 87	45)	( 88	75)
( 89	12)	( 90	37)	( 91	4)	(101	21)	(102	20)
(103	39)	(104	73)	(105	17)	(106	3)	(114	12)
(115	14)	(116	30)	(117	21)	(118	38)	(119	123)
(120	11)	(121	4)	(129	4)	(130	7)	(131	40)
(132	78)	(133	97)	(134	21)	(135	10)	(143	5)
(146	18)	(147	251)	(148	42)	(149	44)	(150	6)
(151	3)	(157	3)	(158	4)	(160	44)	(162	23)
(163	16)	(164	16)	(165	3)	(175	28)	(176	13)
(177	27)	(178	10)	(179	4)	(188	11)	(189	13)
(190	5)	(191	45)	(192	65)	(193	13)	(194	4)
(202	3)	(203	8)	(204	21)	(205	6)	(206	87)
(207	37)	(208	9)	(217	8)	(218	12)	(219	6)
(220	87)	(221	72)	(222	17)	(223	5)	(232	10)
(233	51)	(234	14)	(235	41)	(236	24)	(237	7)
(250	8)	(263	3)	(278	4)	(279	3)	(307	8)
(322	12)	(323	10)	(324	4)	(337	20)	(338	4)
(412	4)								

NAME:13C\_1843.2\_1313EC16\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:184004-11-1

RI:1843

RT:11.419

NUM PEAKS: 29

( 72	23)	( 73	1000)	( 74	79)	( 75	100)	( 89	6)
( 90	16)	(102	10)	(103	40)	(104	57)	(115	9)
(118	21)	(119	59)	(131	26)	(132	62)	(133	64)
(134	13)	(147	221)	(148	39)	(149	25)	(191	44)
(192	259)	(193	43)	(194	17)	(206	349)	(207	66)
(208	24)	(220	129)	(222	12)	(235	5)		

NAME:13C\_1870.4\_1313EC16\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:187004-11-1

RI:1870

RT:11.629



NUM PEAKS: 85

( 70	10)	( 71	11)	( 72	21)	( 73	1000)	( 74	88)
( 75	68)	( 76	3)	( 84	5)	( 85	15)	( 86	5)
( 87	7)	( 90	9)	( 98	4)	( 99	8)	(100	17)
(101	8)	(102	6)	(103	19)	(104	27)	(105	4)
(113	4)	(114	3)	(115	6)	(117	6)	(118	5)
(119	21)	(127	7)	(128	7)	(129	6)	(130	5)
(131	20)	(133	46)	(134	7)	(135	4)	(141	3)
(142	4)	(143	8)	(144	4)	(145	3)	(147	111)
(148	18)	(149	12)	(155	6)	(156	11)	(157	84)
(158	15)	(159	8)	(170	7)	(171	41)	(172	25)
(173	31)	(175	3)	(177	6)	(185	5)	(186	10)
(187	4)	(200	5)	(201	9)	(202	3)	(206	12)
(213	4)	(214	6)	(215	9)	(216	3)	(229	4)
(230	11)	(231	5)	(243	6)	(244	82)	(245	658)
(246	137)	(247	56)	(248	7)	(273	11)	(274	3)
(275	3)	(318	3)	(319	5)	(347	3)	(348	3)
(362	4)	(436	3)	(437	12)	(438	5)	(452	3)

NAME:13C\_1879.2\_1313EC16\_Adenine (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:188005-11-1

RI:1879

RT:11.698

NUM PEAKS: 8

( 73	800)	( 74	88)	(197	207)	(268	190)	(269	1000)
(270	172)	(283	51)	(284	190)				

NAME:13C\_1892.4\_1313EC16\_Tyrosine (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:189006-11-1

RI:1892

RT:11.800

NUM PEAKS: 102

( 70	22)	( 75	321)	( 76	26)	( 77	18)	( 79	3)
( 80	3)	( 81	7)	( 82	13)	( 83	30)	( 84	29)
( 85	25)	( 88	29)	( 91	8)	( 92	5)	( 93	4)
( 94	3)	( 95	7)	( 96	33)	( 97	34)	( 98	56)
( 99	11)	(100	10)	(109	5)	(110	13)	(111	14)
(112	16)	(113	11)	(114	11)	(118	13)	(123	7)
(124	7)	(125	19)	(126	28)	(127	42)	(128	8)
(129	6)	(137	4)	(138	9)	(139	7)	(140	14)
(141	28)	(142	10)	(143	9)	(151	4)	(152	9)
(153	5)	(155	19)	(156	42)	(157	20)	(158	5)
(166	3)	(167	4)	(168	9)	(169	11)	(170	34)
(171	15)	(172	32)	(173	6)	(180	3)	(183	14)
(184	25)	(185	71)	(186	1000)	(187	144)	(188	36)
(197	3)	(198	6)	(199	6)	(200	19)	(201	5)
(202	3)	(203	5)	(212	3)	(213	3)	(214	8)
(215	26)	(216	102)	(217	12)	(221	48)	(223	5)
(226	3)	(227	12)	(228	5)	(229	4)	(231	3)
(245	4)	(260	3)	(264	3)	(272	3)	(273	4)
(290	3)	(295	3)	(296	3)	(301	7)	(302	5)
(307	3)	(317	3)	(318	5)	(319	32)	(320	7)
(321	5)	(334	4)						

NAME:13C\_1940.3\_1313EC16\_Tyrosine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:194002-11-1

RI:1940

RT:12.115

NUM PEAKS: 99

( 70	8)	( 71	6)	( 72	19)	( 73	1000)	( 74	91)
( 75	113)	( 76	7)	( 77	4)	( 82	3)	( 83	7)
( 84	6)	( 85	7)	( 86	4)	( 87	17)	( 88	3)
( 96	10)	( 97	11)	( 98	15)	( 99	3)	(100	4)
(101	167)	(102	27)	(103	12)	(104	7)	(110	5)
(111	5)	(112	7)	(113	3)	(114	3)	(115	3)
(116	4)	(117	6)	(118	4)	(119	3)	(124	3)
(125	5)	(126	6)	(127	4)	(130	3)	(131	15)
(132	52)	(133	25)	(134	6)	(137	3)	(138	4)
(139	3)	(140	5)	(141	10)	(142	3)	(145	3)
(146	4)	(147	109)	(148	19)	(149	10)	(152	4)
(153	3)	(154	6)	(155	7)	(156	19)	(157	4)
(158	3)	(159	3)	(160	4)	(161	5)	(163	9)
(168	5)	(169	4)	(170	15)	(171	8)	(172	9)
(175	4)	(182	3)	(183	5)	(184	10)	(185	8)
(186	69)	(187	10)	(188	4)	(198	3)	(199	4)
(200	16)	(201	3)	(205	6)	(214	3)	(215	8)
(219	14)	(220	594)	(221	105)	(222	50)	(223	5)
(273	7)	(287	9)	(288	55)	(289	10)	(290	4)
(362	13)	(363	6)	(364	3)	(391	6)		

NAME:13C\_1294.2\_1313EC11\_Glycerol (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:129003-11-1

RI:1294

RT:6.336

NUM PEAKS: 46

( 70	4)	( 71	6)	( 72	26)	( 73	1000)	( 74	89)
( 75	84)	( 76	6)	( 87	15)	( 88	7)	( 89	19)
( 90	45)	(101	6)	(102	14)	(103	82)	(104	365)
(105	39)	(106	14)	(118	41)	(119	384)	(120	31)
(132	83)	(134	45)	(147	644)	(148	102)	(149	71)
(150	9)	(160	4)	(161	4)	(164	11)	(175	5)
(176	5)	(177	71)	(178	42)	(179	11)	(180	3)
(192	31)	(206	71)	(207	276)	(208	61)	(209	26)
(220	24)	(221	133)	(222	26)	(223	12)	(265	3)
(296	18)								

NAME:13C\_1326.8\_1313EC11\_Glycine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:133001-11-1

RI:1327

RT:6.720

NUM PEAKS: 59

( 70	12)	( 71	9)	( 72	26)	( 73	1000)	( 74	86)
( 75	61)	( 86	14)	( 87	313)	( 88	26)	( 89	14)
( 99	5)	(100	23)	(101	171)	(102	32)	(103	32)
(104	5)	(105	5)	(113	7)	(114	5)	(115	11)
(116	18)	(117	52)	(118	12)	(119	13)	(129	3)
(130	44)	(131	52)	(132	15)	(133	163)	(134	23)
(135	12)	(147	310)	(148	50)	(149	24)	(159	25)
(160	14)	(161	16)	(162	3)	(173	11)	(174	15)
(175	905)	(176	161)	(177	73)	(178	14)	(188	3)
(190	14)	(191	3)	(204	11)	(205	3)	(206	3)
(247	9)	(248	6)	(249	144)	(250	39)	(251	18)
(252	3)	(278	44)	(279	11)	(280	6)		

NAME:13C\_1340.7\_1313EC11\_Succinic acid (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
CASNO:134001-11-1

RI:1341

RT:6.883

NUM PEAKS: 25

( 72	25)	( 73	546)	( 74	56)	( 75	378)	( 76	27)
( 87	13)	( 88	12)	( 89	9)	(103	13)	(115	8)
(116	8)	(117	9)	(118	25)	(131	22)	(132	95)
(133	51)	(134	11)	(147	1000)	(148	159)	(149	84)
(176	43)	(177	20)	(179	7)	(251	75)	(252	11)

NAME:13C\_1380.4\_1313EC11\_Alanine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:138002-11-1

RI:1380

RT:7.350

NUM PEAKS: 50

( 70	25)	( 71	27)	( 72	36)	( 73	999)	( 85	23)
( 86	22)	( 99	10)	(100	47)	(102	790)	(103	93)
(113	12)	(114	10)	(116	233)	(117	68)	(129	6)
(130	72)	(131	95)	(133	261)	(135	18)	(139	3)
(144	6)	(147	370)	(148	35)	(158	6)	(159	28)
(160	10)	(161	9)	(173	24)	(174	28)	(176	25)
(177	6)	(187	3)	(188	7)	(189	26)	(190	1000)
(191	181)	(192	81)	(193	24)	(203	5)	(233	4)
(247	11)	(248	4)	(263	6)	(264	137)	(265	38)
(266	17)	(292	3)	(293	28)	(294	8)	(295	4)

NAME:13C\_1381.6\_1313EC11\_Serine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:138001-11-1

RI:1382

RT:7.365

NUM PEAKS: 58

( 70	7)	( 71	10)	( 72	27)	( 73	1000)	( 74	104)
( 75	158)	( 76	11)	( 77	6)	( 85	8)	( 86	7)
( 87	22)	( 88	11)	( 89	19)	( 90	9)	(100	10)
(101	122)	(103	22)	(104	63)	(105	10)	(106	3)
(115	14)	(117	25)	(118	70)	(119	26)	(120	4)
(131	29)	(132	46)	(133	73)	(134	24)	(135	8)
(145	7)	(146	11)	(147	163)	(148	31)	(150	6)
(159	5)	(160	7)	(161	5)	(162	6)	(163	7)
(174	9)	(175	10)	(176	9)	(177	5)	(204	7)
(205	28)	(206	318)	(207	57)	(208	25)	(218	3)
(219	16)	(220	169)	(221	37)	(222	15)	(223	3)
(280	17)	(281	5)	(309	8)				

NAME:13C\_1405.3\_1313EC11\_Threonine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:140001-11-1

RI:1405

RT:7.644

NUM PEAKS: 71

( 70	6)	( 71	8)	( 72	27)	( 73	1000)	( 74	100)
( 75	135)	( 76	9)	( 77	5)	( 85	7)	( 86	6)
( 87	28)	( 88	23)	( 89	9)	( 99	3)	(100	5)
(101	93)	(102	167)	(103	43)	(104	18)	(105	7)
(115	12)	(116	7)	(117	45)	(118	20)	(119	219)
(120	19)	(121	8)	(130	13)	(131	141)	(132	73)
(133	92)	(134	30)	(135	9)	(145	8)	(146	7)

(147	153)	(148	30)	(149	23)	(150	3)	(159	6)
(160	16)	(161	14)	(162	6)	(163	6)	(173	4)
(175	8)	(176	3)	(177	3)	(178	5)	(189	7)
(190	3)	(191	5)	(192	7)	(204	3)	(205	51)
(206	17)	(207	8)	(219	5)	(220	86)	(221	309)
(222	60)	(223	26)	(224	3)	(234	6)	(292	3)
(293	53)	(294	16)	(295	30)	(296	8)	(297	3)
(324	9)								

NAME:13C\_1411.1\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:141003-11-1

RI:1411

RT:7.711

NUM PEAKS: 27

( 71	217)	( 73	785)	( 74	54)	( 81	73)	( 85	65)
( 95	18)	( 99	9)	(103	88)	(110	27)	(118	46)
(133	129)	(134	1000)	(135	90)	(136	21)	(147	231)
(148	38)	(149	62)	(150	9)	(157	6)	(191	18)
(192	16)	(207	10)	(279	9)	(280	7)	(294	126)
(295	28)	(296	14)						

NAME:13C\_1440.4\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:144003-11-1

RI:1440

RT:8.056

NUM PEAKS: 54

( 70	8)	( 71	9)	( 72	33)	( 73	1000)	( 74	143)
( 75	437)	( 76	41)	( 77	20)	( 85	6)	( 86	6)
( 87	16)	( 88	12)	( 89	12)	( 90	3)	( 91	6)
(100	5)	(101	13)	(102	67)	(103	23)	(104	27)
(105	4)	(115	6)	(116	7)	(117	20)	(118	262)
(119	143)	(120	18)	(121	4)	(131	31)	(132	279)
(133	59)	(134	17)	(146	7)	(147	171)	(148	46)
(149	22)	(150	4)	(161	4)	(162	39)	(163	455)
(164	40)	(165	17)	(175	6)	(176	8)	(191	5)
(204	16)	(205	3)	(222	13)	(237	29)	(238	5)
(248	8)	(249	38)	(250	6)	(266	10)		

NAME:13C\_1458.8\_1313EC11\_Homoserine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:146001-11-1

RI:1459

RT:8.273

NUM PEAKS: 67

( 70	8)	( 71	11)	( 72	31)	( 73	1000)	( 74	103)
( 75	145)	( 76	12)	( 85	9)	( 86	7)	( 87	23)
( 88	17)	( 89	10)	( 90	4)	( 95	3)	(100	13)
(101	44)	(102	83)	(103	69)	(104	223)	(105	30)
(106	10)	(113	3)	(115	15)	(116	11)	(117	25)
(118	15)	(119	9)	(129	5)	(130	23)	(131	399)
(132	77)	(133	112)	(134	37)	(135	9)	(144	4)
(145	6)	(146	7)	(147	141)	(148	28)	(149	48)
(150	6)	(159	4)	(160	9)	(161	6)	(173	3)
(175	6)	(176	17)	(177	9)	(189	3)	(190	7)
(192	4)	(204	7)	(205	32)	(206	8)	(218	7)
(219	12)	(220	42)	(221	487)	(222	84)	(223	37)
(224	4)	(234	22)	(235	6)	(236	7)	(295	15)
(296	5)	(324	7)						

NAME:13C\_1464.4\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:146003-11-1

RI:1464

RT:8.339

NUM PEAKS: 50

( 70	22)	( 71	24)	( 72	83)	( 73	580)	( 75	242)
( 76	18)	( 77	19)	( 83	4)	( 84	7)	( 85	32)
( 86	46)	( 87	10)	( 88	5)	( 89	4)	( 99	8)
(100	22)	(101	44)	(105	4)	(113	5)	(114	5)
(115	14)	(116	7)	(129	24)	(130	14)	(133	60)
(134	9)	(135	5)	(147	1000)	(148	161)	(149	97)
(150	10)	(151	3)	(159	13)	(160	6)	(173	12)
(175	8)	(190	11)	(191	32)	(192	3)	(203	7)
(218	8)	(219	68)	(220	16)	(221	3)	(263	7)
(264	4)	(293	9)	(294	70)	(295	12)	(296	4)

NAME:13C\_1467.2\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:147003-11-1

RI:1467

RT:8.372

NUM PEAKS: 57

( 71	42)	( 73	1000)	( 74	100)	( 80	7)	( 81	3)
( 82	4)	( 87	49)	( 88	17)	( 89	15)	( 90	7)
( 99	9)	(100	43)	(101	99)	(102	268)	(103	49)
(104	15)	(109	3)	(114	14)	(115	34)	(116	27)
(117	412)	(118	43)	(119	20)	(128	7)	(130	60)
(131	667)	(132	92)	(142	15)	(143	11)	(144	34)
(145	307)	(146	57)	(154	11)	(157	11)	(158	57)
(159	26)	(160	13)	(161	5)	(162	5)	(172	9)
(174	185)	(175	25)	(176	18)	(188	3)	(189	9)
(205	20)	(216	2)	(217	3)	(232	9)	(233	3)
(246	8)	(247	17)	(248	188)	(249	32)	(250	13)
(262	5)	(263	16)						

NAME:13C\_1473.2\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:147002-11-1

RI:1473

RT:8.442

NUM PEAKS: 64

( 74	1000)	( 77	3)	( 78	3)	( 80	3)	( 85	6)
( 86	7)	( 87	5)	( 88	7)	( 89	6)	( 90	50)
( 91	5)	( 94	4)	(101	40)	(102	25)	(105	3)
(110	3)	(114	3)	(115	4)	(116	4)	(117	32)
(122	3)	(130	5)	(131	10)	(132	36)	(142	4)
(145	8)	(146	146)	(157	3)	(158	7)	(159	5)
(160	4)	(162	5)	(163	37)	(164	7)	(174	10)
(176	23)	(186	3)	(188	5)	(191	5)	(194	4)
(210	3)	(215	3)	(220	14)	(228	3)	(245	3)
(280	4)	(323	3)	(335	4)	(349	3)	(360	3)
(385	3)	(386	4)	(387	3)	(410	3)	(423	3)
(431	4)	(434	3)	(441	3)	(459	3)	(495	3)
(524	4)	(532	3)	(535	3)	(542	3)		

NAME:13C\_1481.0\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:148002-11-1

RI:1481

RT:8.534

NUM PEAKS: 16

( 71	19)	( 73	1000)	( 85	62)	( 87	47)	(101	44)
(102	59)	(103	15)	(104	31)	(143	143)	(147	273)
(149	21)	(158	34)	(159	985)	(160	91)	(161	30)
(233	55)								

NAME:13C\_1503.6\_1313EC11\_Erythritol (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:150002-11-1

RI:1504

RT:8.786

NUM PEAKS: 56

( 73	1000)	( 74	74)	( 75	50)	( 76	3)	( 87	4)
( 89	11)	( 90	29)	(103	54)	(104	186)	(105	20)
(106	5)	(115	5)	(116	7)	(119	154)	(120	11)
(121	5)	(131	16)	(132	68)	(133	94)	(134	15)
(135	8)	(145	3)	(146	5)	(147	347)	(148	55)
(149	33)	(150	3)	(177	6)	(178	3)	(189	3)
(191	67)	(192	56)	(193	12)	(194	3)	(205	4)
(206	72)	(207	114)	(208	22)	(209	8)	(218	3)
(219	12)	(220	220)	(221	53)	(222	19)	(223	3)
(235	7)	(279	6)	(280	3)	(295	12)	(296	4)
(309	5)	(310	17)	(311	5)	(312	3)	(324	6)
(325	3)								

NAME:13C\_1506.4\_1313EC11

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:151002-11-1

RI:1506

RT:8.808

NUM PEAKS: 68

( 75	501)	( 76	44)	( 87	77)	( 93	13)	(101	233)
(102	965)	(115	44)	(116	44)	(117	1000)	(122	8)
(123	16)	(130	46)	(131	727)	(145	50)	(157	24)
(158	28)	(159	114)	(161	10)	(185	36)	(186	16)
(190	15)	(197	17)	(199	12)	(203	73)	(204	35)
(210	10)	(218	20)	(227	17)	(235	18)	(238	14)
(242	11)	(243	20)	(244	9)	(246	48)	(247	434)
(248	74)	(249	20)	(250	8)	(269	13)	(270	12)
(275	24)	(276	15)	(281	13)	(282	22)	(305	10)
(313	10)	(325	10)	(339	10)	(346	16)	(347	11)
(350	14)	(356	10)	(360	13)	(361	9)	(368	7)
(376	11)	(405	14)	(426	8)	(436	9)	(440	10)
(448	9)	(453	12)	(454	17)	(464	10)	(518	10)
(524	7)	(542	10)	(553	6)				

NAME:13C\_1513.8\_1313EC11

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:151003-11-1

RI:1514

RT:8.865

NUM PEAKS: 67

( 70	12)	( 72	37)	( 73	1000)	( 74	116)	( 75	276)
( 76	21)	( 77	12)	( 85	14)	( 86	26)	( 87	59)
( 88	909)	( 89	209)	( 90	21)	( 91	15)	(100	14)
(101	79)	(102	147)	(103	23)	(104	28)	(105	32)
(106	5)	(114	4)	(115	18)	(116	8)	(117	49)
(118	17)	(119	10)	(120	19)	(130	7)	(131	102)

(132	53)	(133	60)	(134	11)	(135	5)	(144	46)
(145	10)	(146	13)	(147	159)	(148	36)	(149	17)
(158	7)	(159	7)	(160	118)	(161	18)	(162	38)
(163	17)	(174	8)	(175	5)	(176	27)	(177	5)
(190	9)	(191	55)	(192	885)	(193	87)	(194	34)
(205	22)	(206	7)	(218	4)	(219	3)	(220	17)
(221	7)	(234	31)	(266	14)	(279	23)	(280	4)
(295	10)	(310	10)						

NAME:13C\_1528.8\_1313EC11\_Pyroglutamic acid (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:153002-11-1

RI:1529

RT:8.981

NUM PEAKS: 56

( 70	20)	( 71	33)	( 72	36)	( 73	955)	( 75	138)
( 76	9)	( 77	5)	( 84	7)	( 85	27)	( 86	24)
( 87	21)	( 88	24)	( 95	7)	( 99	5)	(100	7)
(101	24)	(104	4)	(105	4)	(113	6)	(114	4)
(115	31)	(116	8)	(117	25)	(118	6)	(124	14)
(130	5)	(131	22)	(132	9)	(133	38)	(134	6)
(135	3)	(143	4)	(144	29)	(145	11)	(147	167)
(148	27)	(149	17)	(157	3)	(158	16)	(159	42)
(160	1000)	(161	89)	(162	38)	(173	4)	(191	4)
(218	12)	(232	4)	(233	4)	(234	83)	(235	14)
(236	6)	(262	6)	(263	72)	(264	12)	(265	6)
(278	3)								

NAME:13C\_1537.7\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:154002-11-1

RI:1538

RT:9.050

NUM PEAKS: 66

( 72	26)	( 73	543)	( 74	85)	( 75	685)	( 76	58)
( 77	35)	( 86	15)	( 87	66)	( 88	1000)	( 89	26)
( 90	6)	( 91	6)	(100	6)	(101	10)	(102	10)
(103	26)	(104	22)	(105	5)	(115	13)	(116	6)
(117	14)	(118	44)	(119	21)	(120	3)	(131	17)
(132	47)	(133	58)	(134	13)	(135	5)	(143	3)
(144	45)	(145	7)	(146	14)	(147	81)	(148	44)
(149	25)	(150	4)	(158	3)	(159	4)	(160	76)
(161	24)	(162	225)	(163	24)	(164	10)	(176	8)
(177	39)	(178	440)	(179	41)	(180	17)	(190	8)
(191	78)	(192	6)	(193	3)	(206	21)	(207	3)
(218	3)	(234	43)	(235	8)	(236	4)	(252	17)
(253	3)	(263	6)	(280	3)	(281	39)	(282	7)
(283	3)								

NAME:13C\_1561.1\_1313EC11\_Phenylalanine (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:157001-11-1

RI:1561

RT:9.232

NUM PEAKS: 85

( 70	121)	( 72	29)	( 73	590)	( 74	118)	( 75	345)
( 76	35)	( 77	17)	( 81	9)	( 83	87)	( 87	31)
( 89	22)	( 91	36)	( 92	5)	( 96	25)	( 97	29)
( 98	260)	( 99	31)	(100	33)	(101	39)	(102	16)
(104	38)	(108	4)	(110	17)	(111	101)	(113	7)

(116	7)	(118	28)	(121	3)	(124	5)	(125	15)
(126	44)	(127	106)	(128	1000)	(129	4)	(132	186)
(133	42)	(134	19)	(138	3)	(139	18)	(140	5)
(143	9)	(145	5)	(148	414)	(149	40)	(150	22)
(154	4)	(158	4)	(159	63)	(161	7)	(169	9)
(174	3)	(175	14)	(177	4)	(184	13)	(185	13)
(200	3)	(202	8)	(213	33)	(214	6)	(218	4)
(220	56)	(221	15)	(222	63)	(223	9)	(224	5)
(230	3)	(231	19)	(232	3)	(235	3)	(237	4)
(244	3)	(251	7)	(286	3)	(296	3)	(303	3)
(304	3)	(396	5)	(397	4)	(403	3)	(449	3)
(470	3)	(500	3)	(506	3)	(544	3)	(565	3)

NAME:13C\_1575.2\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:157002-11-1

RI:1575

RT:9.341

NUM PEAKS: 57

( 72	34)	( 73	1000)	( 74	121)	( 75	221)	( 76	16)
( 77	8)	( 86	3)	( 89	7)	(102	8)	(103	39)
(105	6)	(111	5)	(115	6)	(118	29)	(119	11)
(131	25)	(132	9)	(133	75)	(134	10)	(135	6)
(145	5)	(146	52)	(147	430)	(148	119)	(149	87)
(150	12)	(151	5)	(161	6)	(162	62)	(163	9)
(175	8)	(176	3)	(177	4)	(178	13)	(191	10)
(192	109)	(193	19)	(194	7)	(207	4)	(221	19)
(222	13)	(235	4)	(236	35)	(237	6)	(266	27)
(267	8)	(280	7)	(281	89)	(282	16)	(283	6)
(294	8)	(308	6)	(310	8)	(355	4)	(383	3)
(384	12)	(385	5)						

NAME:13C\_1580.5\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:158002-11-1

RI:1581

RT:9.382

NUM PEAKS: 104

(109	37)	(110	25)	(111	46)	(112	30)	(122	61)
(123	71)	(124	68)	(125	82)	(126	60)	(127	104)
(128	25)	(185	88)	(186	1000)	(187	69)	(201	90)
(271	13)	(273	13)	(274	22)	(275	84)	(276	11)
(287	20)	(289	11)	(290	89)	(291	20)	(346	12)
(347	17)	(360	14)	(362	24)	(363	18)	(364	28)
(365	31)	(366	12)	(371	19)	(379	10)	(392	14)
(398	19)	(402	20)	(437	15)	(438	18)	(439	19)
(440	12)	(441	19)	(442	16)	(445	22)	(446	11)
(447	25)	(448	10)	(449	19)	(450	40)	(451	27)
(455	31)	(456	21)	(457	29)	(458	29)	(459	30)
(461	39)	(463	27)	(464	23)	(465	27)	(466	30)
(467	38)	(469	29)	(470	25)	(471	20)	(472	24)
(473	43)	(474	32)	(476	28)	(477	16)	(478	29)
(479	17)	(480	18)	(482	31)	(483	18)	(486	21)
(488	26)	(489	20)	(492	18)	(493	12)	(495	26)
(496	33)	(498	20)	(500	17)	(502	14)	(503	13)
(504	27)	(505	22)	(510	15)	(513	15)	(514	29)
(515	20)	(517	18)	(527	15)	(529	16)	(532	21)
(533	14)	(538	14)	(540	17)	(542	20)	(543	16)
(548	17)	(549	21)	(555	14)	(558	10)		



NAME:13C\_1581.9\_1313EC11\_  
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
 CASNO:158003-11-1  
 RI:1582  
 RT:9.393

NUM PEAKS: 86

( 70	8)	( 71	9)	( 72	48)	( 73	1000)	( 74	160)
( 75	299)	( 76	16)	( 85	4)	( 86	6)	( 87	9)
( 91	25)	(100	3)	(101	22)	(102	9)	(103	28)
(104	5)	(105	4)	(115	8)	(116	3)	(117	49)
(118	42)	(119	45)	(130	8)	(131	33)	(133	100)
(134	14)	(135	9)	(145	4)	(146	17)	(147	386)
(148	86)	(149	84)	(150	12)	(151	5)	(161	7)
(162	70)	(163	20)	(164	5)	(175	15)	(176	5)
(177	8)	(178	3)	(190	3)	(191	40)	(192	12)
(193	6)	(204	3)	(205	3)	(206	7)	(207	9)
(219	6)	(220	51)	(221	32)	(222	11)	(223	6)
(234	6)	(235	4)	(236	38)	(237	10)	(238	4)
(249	4)	(250	4)	(263	8)	(264	5)	(265	41)
(266	24)	(267	7)	(280	12)	(281	161)	(282	30)
(283	14)	(293	3)	(294	27)	(295	5)	(296	4)
(308	6)	(309	3)	(353	12)	(354	5)	(355	16)
(356	6)	(357	3)	(383	3)	(384	22)	(385	7)
(386	3)								

NAME:13C\_1623.1\_1313EC11\_  
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
 CASNO:162001-11-1  
 RI:1623  
 RT:9.712

NUM PEAKS: 90

( 70	9)	( 71	13)	( 72	63)	( 73	1000)	( 74	759)
( 75	136)	( 76	14)	( 84	3)	( 85	16)	( 86	12)
( 87	23)	( 88	13)	( 89	37)	( 90	8)	( 91	3)
( 99	5)	(100	15)	(101	54)	(102	80)	(103	118)
(104	24)	(105	11)	(110	3)	(113	3)	(114	6)
(115	13)	(116	15)	(117	88)	(118	26)	(119	28)
(120	3)	(129	4)	(130	26)	(131	83)	(132	59)
(133	42)	(134	10)	(135	3)	(143	3)	(144	15)
(145	37)	(146	650)	(147	215)	(148	66)	(149	17)
(150	3)	(157	4)	(158	17)	(159	16)	(160	8)
(161	11)	(162	61)	(163	13)	(164	6)	(173	10)
(174	18)	(175	14)	(176	7)	(177	4)	(189	5)
(190	9)	(191	10)	(192	6)	(203	6)	(204	3)
(205	6)	(206	42)	(207	8)	(208	3)	(218	7)
(219	14)	(220	47)	(221	15)	(222	5)	(232	4)
(233	4)	(234	4)	(235	8)	(236	8)	(246	4)
(247	4)	(248	31)	(249	25)	(263	8)	(264	11)
(265	3)	(352	3)	(353	26)	(354	8)	(355	4)

NAME:13C\_1652.1\_1313EC11\_  
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
 CASNO:165002-11-1  
 RI:1652  
 RT:9.937

NUM PEAKS: 30

( 73	1000)	( 74	90)	( 85	29)	( 87	28)	(101	53)
(115	94)	(116	75)	(117	31)	(129	25)	(130	62)
(131	57)	(144	26)	(145	14)	(146	115)	(147	159)
(158	27)	(159	26)	(173	81)	(174	40)	(202	21)

76

(203 244) (204 48) (205 17) (217 20) (232 24)  
 (319 17) (320 165) (321 41) (322 17) (335 14)

NAME:13C\_1659.1\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:166002-11-1

RI:1659

RT:9.991

NUM PEAKS: 24

( 70 15) ( 71 66) ( 72 17) ( 73 1000) ( 74 74)  
 ( 90 26) ( 99 14) (103 36) (104 137) (113 15)  
 (119 132) (131 28) (132 39) (133 76) (147 266)  
 (148 36) (161 16) (173 36) (191 58) (203 85)  
 (206 309) (207 116) (208 32) (220 52)

NAME:13C\_1670.3\_1313EC11\_Arabinose methoxyamine (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1670 |RI:1670 |RI:1670

CASNO:167002-11-1

RI:1670

RT:10.078

SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp

NUM PEAKS: 63

( 71 18) ( 73 1000) ( 74 76) ( 88 12) ( 90 17)  
 (103 60) (104 402) (105 56) (106 16) (119 44)  
 (120 9) (121 7) (131 35) (132 57) (133 84)  
 (134 45) (135 9) (147 227) (148 39) (149 25)  
 (150 5) (161 12) (162 43) (163 19) (164 8)  
 (174 7) (177 14) (190 5) (191 61) (192 25)  
 (193 9) (203 10) (205 7) (206 22) (207 28)  
 (208 11) (216 4) (217 16) (219 12) (220 206)  
 (221 43) (222 21) (235 19) (237 5) (240 4)  
 (261 7) (265 11) (275 5) (282 3) (298 4)  
 (307 7) (310 73) (311 22) (312 11) (371 5)  
 (440 6) (477 5) (493 4) (504 4) (522 5)  
 (523 4) (568 3) (584 3)

NAME:13C\_1683.3\_1313EC11\_Aspargine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:168001-11-1

RI:1683

RT:10.179

NUM PEAKS: 90

( 70 10) ( 71 19) ( 72 41) ( 73 1000) ( 74 145)  
 ( 75 265) ( 76 21) ( 77 12) ( 84 5) ( 85 11)  
 ( 86 10) ( 87 17) ( 88 8) ( 89 5) ( 90 7)  
 ( 99 4) (100 18) (101 69) (102 71) (103 19)  
 (115 9) (116 30) (117 54) (118 391) (119 39)  
 (120 18) (128 12) (129 3) (130 12) (131 42)  
 (132 47) (133 102) (134 195) (135 23) (136 7)  
 (143 9) (144 119) (145 21) (146 25) (147 160)  
 (148 29) (149 27) (150 4) (158 4) (159 5)  
 (160 4) (161 5) (162 46) (163 7) (164 3)  
 (172 3) (173 18) (174 9) (175 10) (176 4)  
 (177 3) (188 4) (189 108) (190 32) (191 12)  
 (192 8) (202 5) (203 3) (204 35) (205 11)  
 (206 14) (207 3) (208 3) (216 4) (217 4)  
 (218 20) (219 12) (220 31) (221 7) (222 3)  
 (232 4) (233 10) (234 146) (235 28) (236 13)  
 (246 3) (247 9) (248 4) (249 4) (262 26)  
 (263 8) (264 3) (320 4) (337 7) (352 6)

NAME:13C 1713.4 1313EC11

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1713 |RI:1713

CASNO:171008-11-1

RI:1713

RT:10.412

SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp

NUM PEAKS: 115

( 73 1000)	( 74 100)	( 90 38)	( 92 9)	(104 419)
(105 30)	(106 13)	(107 7)	(118 17)	(119 145)
(120 11)	(132 179)	(137 6)	(165 7)	(177 13)
(180 7)	(191 48)	(192 41)	(193 8)	(194 4)
(206 48)	(207 173)	(208 35)	(209 14)	(213 8)
(220 500)	(221 137)	(222 54)	(223 11)	(224 6)
(225 9)	(227 8)	(238 7)	(240 6)	(248 35)
(249 12)	(253 4)	(265 10)	(267 7)	(270 5)
(279 17)	(280 8)	(282 6)	(283 4)	(284 4)
(286 6)	(289 9)	(294 13)	(295 8)	(296 8)
(308 8)	(309 16)	(310 68)	(311 24)	(312 15)
(313 7)	(314 7)	(316 7)	(321 9)	(322 12)
(323 57)	(324 24)	(325 10)	(326 5)	(329 7)
(330 4)	(336 5)	(339 7)	(344 4)	(346 4)
(347 5)	(349 6)	(353 7)	(355 9)	(359 7)
(377 6)	(383 8)	(388 5)	(390 5)	(391 4)
(392 7)	(393 5)	(398 8)	(399 8)	(400 5)
(402 4)	(406 4)	(407 6)	(408 5)	(410 6)
(413 7)	(416 9)	(427 4)	(431 5)	(452 6)
(454 7)	(458 6)	(459 13)	(464 4)	(466 9)
(476 4)	(479 5)	(482 3)	(488 6)	(490 4)
(493 5)	(498 8)	(502 4)	(503 6)	(508 7)
(509 4)	(524 7)	(558 7)	(567 6)	(596 3)

NAME:13C 1758.0 1313EC11

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:176005-11-1

RI:1758

RT:10.758

NUM PEAKS: 108

( 70 54)	( 71 49)	( 72 115)	( 73 588)	( 74 1000)
( 75 240)	( 76 25)	( 77 13)	( 79 10)	( 80 3)
( 81 3)	( 83 6)	( 84 12)	( 85 92)	( 86 33)
( 87 45)	( 88 46)	( 89 129)	( 90 23)	( 91 6)
( 92 3)	( 93 5)	( 94 3)	( 95 3)	( 97 4)
( 98 7)	( 99 31)	(100 145)	(101 43)	(102 33)
(103 14)	(104 26)	(105 7)	(106 3)	(109 3)
(111 4)	(112 4)	(113 9)	(114 7)	(115 28)
(116 25)	(117 26)	(118 29)	(119 6)	(124 3)
(125 3)	(126 3)	(127 7)	(128 33)	(129 40)
(130 13)	(131 27)	(132 58)	(133 39)	(134 7)
(135 4)	(140 3)	(141 4)	(142 3)	(143 24)
(144 23)	(145 42)	(147 55)	(148 26)	(149 12)
(150 3)	(156 5)	(157 8)	(158 10)	(159 19)
(160 12)	(161 10)	(162 22)	(163 7)	(164 3)
(169 4)	(171 4)	(172 18)	(173 35)	(174 11)
(177 71)	(178 6)	(179 5)	(187 8)	(188 38)
(189 364)	(190 40)	(191 44)	(192 14)	(193 3)
(202 5)	(203 3)	(211 6)	(215 4)	(216 3)
(217 9)	(218 4)	(219 3)	(229 8)	(230 3)
(263 10)	(264 4)	(275 4)	(285 3)	(290 3)
(291 3)	(292 8)	(307 3)		

NAME:13C\_1763.8\_1313EC11\_Ornithine (3TMS); Arginine {BP} (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:176006-11-1

RI:1764

RT:10.803

NUM PEAKS: 81

( 70	11)	( 71	13)	( 72	84)	( 73	1000)	( 74	297)
( 75	200)	( 76	18)	( 77	7)	( 84	4)	( 85	19)
( 86	17)	( 87	211)	( 88	39)	( 89	13)	( 90	16)
( 91	4)	( 99	5)	(100	28)	(101	102)	(102	47)
(103	40)	(104	13)	(105	4)	(113	8)	(114	12)
(115	18)	(116	23)	(117	32)	(118	18)	(119	11)
(129	5)	(130	78)	(131	77)	(132	41)	(133	44)
(134	7)	(135	3)	(143	3)	(144	11)	(145	15)
(146	261)	(147	141)	(148	48)	(149	16)	(150	3)
(157	5)	(158	9)	(159	29)	(160	8)	(161	24)
(162	39)	(163	5)	(173	20)	(174	35)	(175	707)
(176	127)	(177	75)	(178	8)	(190	15)	(191	200)
(192	32)	(193	9)	(203	11)	(204	4)	(205	3)
(206	5)	(218	4)	(219	5)	(220	29)	(221	7)
(222	3)	(248	12)	(249	55)	(250	10)	(251	4)
(263	16)	(264	5)	(352	4)	(353	32)	(354	10)
(355	4)								

NAME:13C\_1774.2\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:177004-11-1

RI:1774

RT:10.884

NUM PEAKS: 50

( 72	17)	( 73	1000)	( 74	81)	( 75	72)	( 76	10)
( 86	12)	( 90	6)	(100	4)	(114	5)	(115	9)
(116	8)	(119	14)	(131	33)	(132	38)	(133	51)
(144	3)	(145	9)	(146	30)	(147	249)	(148	41)
(149	31)	(150	4)	(161	6)	(164	6)	(174	23)
(178	3)	(192	29)	(205	3)	(206	14)	(219	17)
(220	481)	(221	105)	(222	43)	(223	6)	(235	45)
(236	11)	(237	4)	(248	7)	(249	6)	(250	3)
(261	3)	(262	13)	(263	4)	(295	6)	(308	13)
(309	4)	(322	4)	(455	4)	(456	12)	(457	6)

NAME:13C\_1794.5\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:179002-11-1

RI:1795

RT:11.041

NUM PEAKS: 162

( 70	14)	( 72	26)	( 75	306)	( 76	47)	( 80	8)
( 82	13)	( 85	28)	( 86	32)	( 87	461)	( 90	19)
( 92	13)	( 95	16)	(100	20)	(101	158)	(103	58)
(113	26)	(122	10)	(124	13)	(126	10)	(129	16)
(130	39)	(141	10)	(143	14)	(144	19)	(146	33)
(154	12)	(160	115)	(161	74)	(171	23)	(175	1000)
(176	168)	(177	62)	(178	27)	(180	10)	(181	13)
(182	16)	(187	19)	(188	16)	(191	91)	(192	23)
(196	14)	(199	9)	(212	11)	(213	15)	(214	15)
(215	10)	(224	11)	(226	8)	(232	10)	(233	18)
(239	12)	(241	7)	(244	12)	(245	12)	(247	15)
(250	15)	(256	13)	(257	14)	(258	16)	(259	12)

(260	21)	(262	21)	(266	13)	(269	10)	(272	10)
(273	7)	(274	11)	(275	10)	(276	12)	(277	19)
(288	18)	(289	7)	(290	19)	(291	7)	(296	12)
(308	13)	(309	9)	(311	10)	(312	8)	(316	11)
(317	18)	(318	23)	(322	13)	(324	11)	(332	18)
(335	14)	(337	14)	(339	10)	(340	8)	(346	9)
(349	18)	(350	81)	(351	30)	(352	15)	(357	10)
(369	11)	(370	9)	(372	13)	(373	13)	(374	13)
(379	11)	(380	12)	(383	9)	(384	15)	(385	9)
(386	22)	(390	12)	(398	8)	(404	16)	(406	8)
(407	13)	(413	9)	(414	14)	(421	14)	(423	25)
(424	20)	(426	9)	(427	17)	(433	9)	(435	8)
(438	12)	(447	9)	(453	12)	(456	13)	(463	11)
(464	13)	(466	9)	(468	9)	(470	14)	(471	12)
(476	12)	(477	21)	(478	11)	(480	12)	(481	12)
(482	14)	(483	14)	(487	10)	(490	14)	(494	8)
(496	12)	(503	19)	(510	17)	(511	12)	(513	17)
(515	11)	(517	11)	(522	15)	(524	17)	(525	9)
(530	11)	(534	13)	(537	12)	(546	9)	(547	9)
(549	9)	(555	8)	(565	11)	(567	11)	(571	12)
(577	5)	(593	4)						

NAME:13C\_1809.0\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:181005-11-1

RI:1809

RT:11.153

NUM PEAKS: 13

( 73	1000)	(118	18)	(119	58)	(131	53)	(133	66)
(147	162)	(148	33)	(192	423)	(193	87)	(206	721)
(207	121)	(208	38)	(220	107)				

NAME:13C\_1813.5\_1313EC11\_Glyceric acid-3-phosphate (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:181003-11-1

RI:1814

RT:11.189

NUM PEAKS: 40

( 72	21)	( 73	1000)	( 74	81)	( 75	106)	( 77	14)
(103	96)	(105	12)	(117	8)	(118	29)	(119	23)
(121	8)	(131	22)	(133	111)	(134	13)	(135	35)
(147	233)	(148	40)	(149	21)	(181	18)	(191	24)
(193	20)	(195	17)	(211	130)	(212	19)	(225	18)
(227	101)	(228	15)	(255	8)	(285	15)	(299	137)
(300	35)	(315	47)	(316	14)	(358	12)	(359	68)
(360	18)	(361	8)	(387	32)	(388	14)	(462	15)

NAME:13C\_1852.0\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:185004-11-1

RI:1852

RT:11.487

NUM PEAKS: 33

( 75	1000)	( 76	100)	( 77	67)	( 81	48)	(118	188)
(119	463)	(129	239)	(131	85)	(132	469)	(134	270)
(135	49)	(143	33)	(145	114)	(150	20)	(153	19)
(163	32)	(192	29)	(205	47)	(208	25)	(213	22)
(239	12)	(286	49)	(299	109)	(312	19)	(334	18)
(379	20)	(380	13)	(382	16)	(412	17)	(413	17)
(441	22)	(462	12)	(483	17)				

NAME:13C\_1878.9\_1313EC11\_alpha-D-Methylglucopyranoside (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:188006-11-1

RI:1879

RT:11.695

NUM PEAKS: 45

( 73 1000)	( 74 100)	( 76 41)	( 77 11)	( 93 16)
( 96 2)	( 97 2)	(100 6)	(113 3)	(118 35)
(121 13)	(122 5)	(123 3)	(127 2)	(134 235)
(135 26)	(136 8)	(150 39)	(151 4)	(167 13)
(168 3)	(169 3)	(171 2)	(174 17)	(179 2)
(189 9)	(196 2)	(197 6)	(205 20)	(206 500)
(223 22)	(224 3)	(245 9)	(246 2)	(247 2)
(250 3)	(268 7)	(269 33)	(270 6)	(271 2)
(277 4)	(284 5)	(293 10)	(351 2)	(383 4)

NAME:13C\_1882.2\_1313EC11\_Mannose methoxyamine (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:188002-11-1

RI:1882

RT:11.721

NUM PEAKS: 62

( 70 6)	( 72 18)	( 73 1000)	( 74 84)	( 75 136)
( 87 37)	( 88 20)	( 90 13)	(101 29)	(102 16)
(105 27)	(114 3)	(115 24)	(117 18)	(119 78)
(120 5)	(130 15)	(131 75)	(132 112)	(133 43)
(144 8)	(145 11)	(147 343)	(148 37)	(160 70)
(161 116)	(162 170)	(163 26)	(164 7)	(178 6)
(203 10)	(207 173)	(208 20)	(209 13)	(210 3)
(211 7)	(216 4)	(219 13)	(232 5)	(233 29)
(234 49)	(235 14)	(236 7)	(251 3)	(260 3)
(278 6)	(294 22)	(295 5)	(296 5)	(299 11)
(308 3)	(321 4)	(322 31)	(323 167)	(324 51)
(325 20)	(341 4)	(359 8)	(370 4)	(373 5)
(469 3)	(514 4)			

NAME:13C\_1888.8\_1313EC11

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:189005-11-1

RI:1889

RT:11.772

NUM PEAKS: 5

(192 571)	(193 87)	(194 40)	(206 1000)	(441 7)
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NAME:13C\_1893.5\_1313EC11\_Glucose methoxyamine (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:189002-11-1

RI:1894

RT:11.808

NUM PEAKS: 91

( 70 6)	( 71 6)	( 72 17)	( 73 1000)	( 74 98)
( 75 91)	( 76 4)	( 85 5)	( 86 10)	( 87 33)
( 88 6)	( 89 45)	( 90 33)	( 91 5)	(100 3)
(101 22)	(102 16)	(103 42)	(104 131)	(105 53)
(106 10)	(114 4)	(115 11)	(116 24)	(117 15)
(118 14)	(119 126)	(120 11)	(121 5)	(129 4)
(130 10)	(131 46)	(132 186)	(133 106)	(134 39)
(135 10)	(144 4)	(145 12)	(146 24)	(147 486)
(148 82)	(149 48)	(150 6)	(159 4)	(160 9)

(161	126)	(162	232)	(163	49)	(164	17)	(173	6)
(174	6)	(175	4)	(176	7)	(177	9)	(178	6)
(189	4)	(190	7)	(191	52)	(193	7)	(203	6)
(204	5)	(205	6)	(207	240)	(208	47)	(209	22)
(218	5)	(219	18)	(220	131)	(221	38)	(222	15)
(223	3)	(232	3)	(233	39)	(234	19)	(235	23)
(236	8)	(237	3)	(247	3)	(248	7)	(249	6)
(250	4)	(261	3)	(264	3)	(275	4)	(306	3)
(308	6)	(310	5)	(322	14)	(323	188)	(368	5)
(380	3)								

NAME:13C\_1914.8\_1313EC11\_Glucose methoxyamine {BP} (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:191001-11-1

RI:1915

RT:11.953

NUM PEAKS: 68

( 73	1000)	( 75	54)	( 87	18)	( 89	67)	( 90	29)
( 91	5)	(101	17)	(103	31)	(104	208)	(105	37)
(106	10)	(118	11)	(119	92)	(120	10)	(121	4)
(132	126)	(133	76)	(134	38)	(135	9)	(145	5)
(147	332)	(148	54)	(149	35)	(150	4)	(161	85)
(162	133)	(163	31)	(164	10)	(173	4)	(177	8)
(178	6)	(190	6)	(191	36)	(192	16)	(193	5)
(203	3)	(204	3)	(205	5)	(206	40)	(207	188)
(208	36)	(209	16)	(219	8)	(220	86)	(221	24)
(222	10)	(233	26)	(234	8)	(235	22)	(236	7)
(237	9)	(248	5)	(249	4)	(250	3)	(274	3)
(278	5)	(279	8)	(280	3)	(294	10)	(295	3)
(308	5)	(309	3)	(310	5)	(322	12)	(323	159)
(324	46)	(325	23)	(326	4)				

NAME:13C\_1931.9\_1313EC11\_Sorbitol (6TMS); Glucitol (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:193001-11-1

RI:1932

RT:12.062

NUM PEAKS: 79

( 71	4)	( 72	20)	( 73	1000)	( 74	85)	( 75	68)
( 76	4)	( 87	17)	( 88	5)	( 89	9)	( 90	28)
( 91	3)	(102	11)	(103	33)	(104	179)	(105	19)
(106	7)	(115	5)	(116	5)	(117	7)	(118	10)
(119	107)	(120	8)	(121	4)	(131	27)	(132	92)
(133	73)	(134	12)	(135	6)	(145	4)	(146	14)
(147	344)	(148	59)	(149	35)	(150	4)	(160	8)
(161	73)	(162	7)	(163	5)	(164	4)	(177	7)
(178	3)	(189	10)	(191	39)	(192	35)	(193	9)
(205	6)	(206	50)	(207	157)	(208	29)	(209	12)
(219	6)	(220	165)	(221	40)	(222	16)	(223	3)
(233	16)	(234	7)	(235	17)	(236	3)	(261	7)
(264	5)	(279	8)	(280	4)	(294	8)	(308	6)
(309	8)	(310	26)	(311	7)	(312	3)	(322	12)
(323	127)	(324	36)	(325	17)	(326	3)	(336	10)
(337	3)	(351	6)	(425	3)	(426	4)		

NAME:13C\_1956.1\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:196004-11-1

RI:1956

RT:12.216

## NUM PEAKS: 94

( 70	4)	( 72	20)	( 73	1000)	( 74	92)	( 75	122)
( 76	9)	( 77	9)	( 86	29)	( 87	12)	( 88	6)
( 89	35)	( 90	26)	( 91	7)	(100	3)	(101	12)
(102	13)	(103	32)	(104	99)	(105	21)	(106	5)
(114	6)	(115	17)	(116	9)	(117	11)	(118	14)
(119	59)	(120	6)	(129	4)	(130	7)	(131	28)
(132	116)	(133	74)	(134	18)	(135	8)	(144	8)
(145	12)	(146	19)	(147	174)	(148	36)	(149	46)
(150	5)	(151	3)	(158	5)	(159	5)	(160	15)
(162	18)	(163	21)	(164	4)	(173	7)	(174	57)
(175	32)	(176	12)	(177	12)	(178	4)	(190	10)
(191	36)	(192	24)	(193	6)	(203	3)	(204	3)
(205	6)	(206	57)	(207	21)	(208	7)	(218	4)
(219	12)	(220	226)	(221	43)	(222	30)	(223	5)
(232	3)	(233	6)	(234	6)	(235	6)	(246	3)
(247	7)	(248	32)	(249	12)	(250	5)	(251	5)
(264	5)	(265	3)	(277	17)	(278	4)	(294	4)
(308	4)	(323	7)	(336	6)	(337	13)	(338	5)
(366	7)	(367	41)	(368	13)	(369	6)		

NAME:13C\_1973.5\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:197002-11-1

RI:1974

RT:12.326

## NUM PEAKS: 61

( 70	4)	( 72	19)	( 73	1000)	( 74	86)	( 75	97)
( 77	3)	( 86	9)	( 87	9)	( 88	4)	( 90	13)
(101	5)	(102	8)	(103	34)	(104	59)	(105	9)
(106	3)	(114	3)	(115	8)	(117	8)	(118	17)
(119	36)	(120	3)	(131	27)	(132	67)	(133	67)
(134	11)	(135	6)	(145	4)	(146	17)	(147	227)
(148	37)	(160	7)	(161	11)	(164	3)	(176	3)
(177	4)	(178	3)	(189	3)	(191	47)	(192	270)
(193	47)	(194	20)	(204	8)	(205	13)	(206	441)
(207	81)	(208	36)	(209	4)	(220	84)	(221	28)
(222	11)	(234	3)	(235	9)	(236	4)	(248	6)
(294	6)	(308	6)	(322	3)	(323	4)	(351	3)
(441	3)								

NAME:13C\_1999.9\_1313EC11\_Gluconic acid (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:200001-11-1

RI:2000

RT:12.494

## NUM PEAKS: 62

( 73	1000)	( 81	19)	( 82	28)	( 90	16)	( 96	19)
( 98	15)	(103	22)	(104	95)	(105	13)	(109	5)
(112	12)	(119	66)	(124	6)	(125	22)	(127	4)
(132	63)	(133	65)	(134	11)	(135	8)	(147	349)
(148	57)	(149	38)	(161	26)	(168	5)	(191	39)
(192	23)	(206	40)	(207	68)	(208	13)	(209	7)
(220	87)	(221	28)	(222	17)	(233	7)	(248	9)
(249	7)	(261	4)	(266	4)	(279	14)	(294	67)
(295	23)	(296	11)	(308	29)	(309	13)	(310	11)
(311	5)	(323	29)	(336	18)	(337	64)	(338	23)
(339	12)	(340	6)	(344	5)	(346	6)	(350	5)
(364	8)	(365	14)	(428	5)	(454	4)	(505	7)
(528	4)	(550	4)						



NAME:13C\_2026.0\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:203003-11-1

RI:2026

RT:12.660

NUM PEAKS: 53

( 71	4)	( 73	1000)	( 74	74)	( 86	6)	( 89	41)
( 90	15)	( 91	6)	(101	39)	(103	29)	(104	46)
(105	13)	(131	20)	(133	51)	(145	4)	(146	12)
(147	175)	(148	18)	(149	45)	(150	4)	(160	4)
(161	27)	(162	5)	(164	3)	(173	7)	(174	14)
(175	4)	(176	3)	(189	3)	(191	29)	(192	20)
(193	5)	(205	8)	(206	325)	(207	73)	(208	28)
(209	4)	(219	5)	(220	74)	(221	83)	(222	20)
(223	7)	(233	6)	(234	4)	(235	15)	(236	4)
(249	4)	(264	6)	(294	3)	(308	4)	(322	6)
(323	56)	(324	16)	(325	7)				

NAME:13C\_2028.6\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:203002-11-1

RI:2029

RT:12.676

NUM PEAKS: 88

( 70	33)	( 71	34)	( 72	236)	( 74	190)	( 75	1000)
( 76	82)	( 77	52)	( 82	3)	( 83	29)	( 84	19)
( 85	101)	( 86	45)	( 87	185)	( 88	114)	( 89	168)
( 93	3)	( 96	3)	( 97	5)	( 98	35)	( 99	12)
(100	60)	(102	213)	(103	102)	(104	101)	(106	14)
(113	15)	(114	6)	(115	32)	(116	38)	(117	77)
(118	146)	(119	527)	(120	42)	(121	20)	(126	3)
(127	4)	(128	22)	(129	9)	(130	32)	(131	42)
(132	468)	(134	188)	(135	31)	(136	8)	(137	3)
(141	3)	(142	4)	(143	19)	(144	20)	(145	18)
(146	35)	(148	164)	(150	10)	(157	3)	(158	12)
(159	10)	(160	23)	(162	39)	(163	47)	(164	5)
(165	5)	(175	15)	(176	21)	(177	28)	(178	16)
(179	4)	(181	3)	(188	3)	(189	6)	(190	16)
(193	8)	(194	4)	(204	3)	(237	6)	(238	6)
(239	3)	(250	3)	(251	5)	(252	29)	(253	5)
(254	4)	(301	3)	(326	22)	(327	106)	(328	15)
(329	4)	(341	3)	(342	10)				

NAME:13C\_2039.3\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:204003-11-1

RI:2039

RT:12.745

NUM PEAKS: 56

( 73	1000)	( 74	83)	( 87	116)	(101	75)	(102	49)
(115	34)	(130	113)	(131	46)	(133	47)	(145	24)
(147	143)	(149	20)	(152	14)	(159	23)	(171	9)
(173	37)	(175	313)	(176	58)	(177	53)	(183	15)
(189	18)	(190	18)	(195	9)	(203	57)	(216	18)
(217	33)	(218	346)	(219	65)	(222	10)	(231	18)
(242	16)	(262	16)	(275	16)	(277	17)	(292	41)
(293	21)	(345	15)	(346	7)	(378	17)	(379	39)
(396	16)	(425	12)	(432	11)	(438	8)	(449	12)
(453	15)	(462	14)	(463	17)	(473	16)	(476	13)

(491 15) (508 17) (557 9) (566 14) (571 8)  
(585 4)

NAME:13C\_2048.0\_1313EC11\_Hexadecanoic acid (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:205001-11-1

RI:2048

RT:12.800

NUM PEAKS: 86

( 70 8) ( 72 95) ( 73 1000) ( 74 227) ( 75 996)  
( 76 109) ( 77 53) ( 85 23) ( 86 10) ( 87 82)  
( 88 37) ( 89 108) ( 90 12) ( 91 15) (100 22)  
(101 12) (102 76) (103 42) (104 65) (105 6)  
(106 28) (107 3) (115 9) (118 161) (119 904)  
(120 71) (121 35) (130 13) (132 489) (133 68)  
(134 607) (135 85) (136 26) (137 3) (140 4)  
(147 53) (148 223) (149 34) (150 11) (160 7)  
(161 6) (162 16) (163 28) (164 11) (175 4)  
(177 22) (178 9) (179 6) (192 32) (193 24)  
(194 8) (206 4) (207 14) (208 50) (209 7)  
(210 3) (211 3) (220 3) (222 10) (223 8)  
(224 3) (233 3) (237 8) (238 11) (239 3)  
(252 5) (253 11) (267 3) (268 6) (282 7)  
(283 3) (284 6) (297 4) (298 12) (299 11)  
(300 3) (315 4) (327 10) (328 38) (329 194)  
(330 28) (331 7) (343 6) (344 21) (345 3)  
(387 4)

NAME:13C\_2087.2\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:209004-11-1

RI:2087

RT:13.049

NUM PEAKS: 65

( 71 8) ( 72 21) ( 73 1000) ( 74 86) ( 75 87)  
( 76 7) ( 85 9) ( 86 14) ( 87 10) ( 89 71)  
( 90 23) ( 91 7) (101 45) (102 15) (103 31)  
(104 65) (105 16) (106 4) (114 5) (116 6)  
(117 13) (118 16) (119 42) (131 23) (132 74)  
(133 49) (134 12) (145 8) (146 17) (147 157)  
(148 32) (149 50) (150 7) (160 8) (161 32)  
(162 10) (163 9) (164 5) (173 10) (174 12)  
(176 6) (187 3) (192 19) (193 4) (202 3)  
(205 7) (206 362) (207 84) (208 30) (209 5)  
(220 75) (221 92) (222 22) (223 7) (233 9)  
(234 6) (235 18) (248 11) (249 4) (264 5)  
(294 7) (322 9) (323 69) (324 20) (325 9)

NAME:13C\_2063.4\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:206001-11-1

RI:2063

RT:12.898

NUM PEAKS: 296

( 70 45) ( 71 26) ( 72 65) ( 74 180) ( 75 213)  
( 79 27) ( 80 24) ( 81 33) ( 86 33) ( 87 255)  
( 89 32) ( 91 29) ( 95 34) ( 99 33) (100 24)  
(101 131) (103 110) (105 33) (106 48) (109 37)  
(112 26) (113 32) (114 36) (115 62) (116 33)  
(117 99) (118 52) (119 205) (120 42) (122 42)

(125	21)	(126	20)	(128	33)	(130	37)	(131	72)
(132	33)	(133	116)	(135	31)	(137	25)	(139	26)
(140	51)	(141	19)	(142	25)	(143	28)	(144	40)
(145	42)	(147	308)	(148	107)	(149	59)	(150	23)
(151	45)	(153	31)	(157	31)	(159	31)	(160	60)
(161	48)	(164	31)	(165	42)	(166	22)	(167	21)
(168	24)	(169	27)	(171	23)	(173	40)	(174	56)
(175	1000)	(176	223)	(177	161)	(178	42)	(179	52)
(180	22)	(182	29)	(186	22)	(188	25)	(189	66)
(192	47)	(201	49)	(205	39)	(206	23)	(208	19)
(209	26)	(210	22)	(211	69)	(212	60)	(213	35)
(214	24)	(215	39)	(217	29)	(219	31)	(221	32)
(222	27)	(224	41)	(225	26)	(226	30)	(227	41)
(230	29)	(231	37)	(232	23)	(233	28)	(234	26)
(235	37)	(236	47)	(237	33)	(239	21)	(243	22)
(246	33)	(247	59)	(248	91)	(249	29)	(254	33)
(255	33)	(256	33)	(257	36)	(261	20)	(262	42)
(263	130)	(264	46)	(265	38)	(266	41)	(268	30)
(269	27)	(271	26)	(273	18)	(274	43)	(275	37)
(276	29)	(277	20)	(278	31)	(279	37)	(281	44)
(282	25)	(289	22)	(291	20)	(292	36)	(295	22)
(297	28)	(299	63)	(303	24)	(305	34)	(310	29)
(312	24)	(313	42)	(314	24)	(315	61)	(318	40)
(321	30)	(322	21)	(323	27)	(324	48)	(325	43)
(328	36)	(329	35)	(330	38)	(332	30)	(334	39)
(335	17)	(337	38)	(338	44)	(340	26)	(341	34)
(344	22)	(346	18)	(347	31)	(350	23)	(355	29)
(356	49)	(357	27)	(359	24)	(360	24)	(361	29)
(364	25)	(365	29)	(371	30)	(374	38)	(376	32)
(377	20)	(383	20)	(384	50)	(385	50)	(386	29)
(387	21)	(388	28)	(389	33)	(390	29)	(394	25)
(395	33)	(397	35)	(398	25)	(399	29)	(401	21)
(404	22)	(405	26)	(406	40)	(407	31)	(408	31)
(409	19)	(411	24)	(412	25)	(414	32)	(417	21)
(418	36)	(419	22)	(420	23)	(422	31)	(423	34)
(424	27)	(425	26)	(426	29)	(427	29)	(428	21)
(431	26)	(432	23)	(433	24)	(434	32)	(435	22)
(437	23)	(438	30)	(441	22)	(442	29)	(446	34)
(448	33)	(449	16)	(451	20)	(453	31)	(454	49)
(455	98)	(456	50)	(457	41)	(459	21)	(460	25)
(461	39)	(462	37)	(465	29)	(466	25)	(467	47)
(468	25)	(469	27)	(472	34)	(473	37)	(477	22)
(480	25)	(481	25)	(482	38)	(483	30)	(485	27)
(487	27)	(488	35)	(492	30)	(493	35)	(494	28)
(495	34)	(496	30)	(498	26)	(499	42)	(500	25)
(501	44)	(503	22)	(504	36)	(508	30)	(509	26)
(510	36)	(514	30)	(515	23)	(516	23)	(517	35)
(518	32)	(519	30)	(521	22)	(522	29)	(523	22)
(524	29)	(526	25)	(527	22)	(528	37)	(529	33)
(531	26)	(533	34)	(535	56)	(536	45)	(537	36)
(538	26)	(539	19)	(542	30)	(546	35)	(547	52)
(550	24)	(554	25)	(560	18)	(564	30)	(565	15)
(566	21)	(570	23)	(571	21)	(579	22)	(583	14)
(592	14)								

NAME:13C\_2025.7\_1313EC16\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:203004-11-1

RI:2026

RT:12.686

NUM PEAKS: 343

( 70	22)	( 71	55)	( 72	44)	( 73	1000)	( 74	58)
( 75	317)	( 76	5)	( 77	20)	( 78	11)	( 79	11)
( 80	8)	( 81	8)	( 82	4)	( 83	17)	( 84	38)
( 85	50)	( 86	29)	( 87	24)	( 88	17)	( 90	7)
( 92	9)	( 93	6)	( 94	3)	( 96	5)	( 97	7)
( 98	11)	( 99	20)	(100	35)	(101	5)	(102	41)
(103	40)	(104	11)	(105	18)	(106	9)	(107	21)
(109	4)	(111	4)	(112	9)	(113	3)	(114	14)
(115	35)	(116	27)	(117	10)	(118	17)	(119	38)
(122	12)	(123	15)	(127	11)	(129	10)	(130	8)
(131	59)	(132	79)	(133	96)	(135	18)	(137	22)
(138	4)	(141	9)	(142	3)	(143	10)	(144	5)
(145	11)	(146	20)	(147	194)	(148	46)	(149	13)
(150	4)	(151	9)	(153	16)	(154	6)	(155	15)
(156	17)	(157	8)	(162	18)	(164	4)	(165	12)
(167	18)	(169	5)	(170	4)	(171	3)	(172	14)
(173	22)	(174	155)	(175	31)	(176	12)	(177	6)
(178	7)	(179	3)	(181	16)	(182	4)	(183	20)
(185	4)	(187	7)	(188	15)	(189	43)	(190	8)
(191	5)	(192	3)	(193	20)	(194	7)	(195	7)
(196	7)	(197	10)	(199	3)	(200	10)	(202	5)
(203	9)	(204	3)	(205	6)	(210	10)	(211	106)
(212	23)	(213	3)	(214	10)	(215	3)	(216	15)
(217	5)	(218	15)	(219	13)	(223	4)	(224	8)
(225	16)	(226	9)	(227	35)	(228	13)	(229	8)
(230	5)	(231	3)	(233	7)	(234	6)	(240	4)
(241	15)	(242	4)	(243	24)	(244	6)	(245	7)
(246	4)	(247	69)	(248	190)	(249	54)	(250	11)
(251	10)	(252	8)	(253	6)	(254	9)	(255	10)
(256	10)	(257	8)	(259	4)	(260	3)	(261	5)
(262	27)	(263	134)	(264	34)	(265	8)	(266	3)
(267	10)	(268	6)	(269	6)	(273	4)	(276	7)
(277	5)	(278	11)	(279	18)	(280	5)	(282	13)
(283	8)	(284	8)	(285	4)	(289	3)	(290	12)
(291	8)	(292	5)	(293	7)	(294	5)	(295	3)
(296	6)	(297	5)	(298	14)	(299	122)	(300	56)
(301	19)	(302	7)	(303	9)	(304	3)	(307	6)
(308	5)	(309	6)	(313	13)	(314	14)	(315	101)
(316	29)	(317	13)	(320	3)	(325	16)	(326	19)
(327	21)	(330	3)	(332	3)	(333	5)	(334	9)
(335	3)	(336	11)	(337	9)	(338	6)	(341	12)
(342	16)	(345	3)	(346	13)	(347	8)	(348	6)
(349	11)	(350	7)	(352	9)	(353	6)	(354	3)
(355	6)	(356	10)	(357	8)	(360	4)	(361	14)
(362	7)	(363	3)	(364	18)	(365	12)	(366	3)
(368	4)	(369	8)	(371	9)	(372	5)	(373	3)
(374	3)	(376	4)	(382	3)	(383	3)	(388	3)
(389	10)	(391	3)	(398	6)	(399	6)	(401	9)
(402	6)	(403	5)	(404	4)	(405	3)	(407	4)
(408	5)	(409	4)	(410	9)	(411	15)	(412	6)
(414	5)	(415	10)	(420	8)	(421	11)	(422	3)
(423	3)	(427	6)	(428	7)	(430	7)	(431	13)
(432	10)	(433	9)	(434	3)	(436	6)	(441	7)
(444	5)	(445	3)	(446	7)	(452	7)	(453	6)
(454	3)	(455	7)	(456	6)	(457	10)	(458	9)
(461	8)	(462	14)	(468	4)	(469	11)	(471	8)
(472	3)	(473	7)	(477	3)	(478	11)	(480	4)
(483	4)	(484	6)	(487	4)	(488	5)	(489	7)
(490	9)	(491	8)	(492	6)	(494	7)	(497	14)

87

(501	10)	(502	10)	(504	4)	(506	8)	(507	5)
(508	11)	(509	3)	(510	3)	(512	5)	(513	4)
(514	4)	(515	4)	(519	8)	(520	7)	(522	5)
(527	6)	(530	6)	(532	7)	(533	13)	(535	5)
(537	4)	(538	4)	(539	3)	(543	9)	(544	8)
(545	4)	(547	5)	(550	5)	(551	4)	(552	7)
(553	3)	(557	5)	(558	7)	(559	5)	(560	6)
(566	4)	(567	3)	(568	5)	(569	5)	(571	10)
(572	5)	(573	4)	(574	3)	(575	4)	(580	6)
(581	5)	(582	5)	(597	3)				

NAME:13C\_2003.6\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:200002-11-1

RI:2004

RT:12.518

NUM PEAKS: 114

( 72	48)	( 73	434)	( 74	140)	( 75	206)	( 76	23)
( 77	11)	( 86	16)	( 87	216)	( 88	32)	( 89	13)
( 94	5)	( 99	11)	(100	68)	(101	111)	(102	42)
(103	22)	(113	10)	(114	7)	(115	34)	(116	31)
(117	50)	(118	51)	(123	5)	(129	15)	(130	72)
(131	114)	(134	7)	(135	7)	(137	5)	(143	27)
(144	16)	(145	12)	(146	126)	(150	6)	(152	4)
(156	9)	(157	13)	(158	7)	(159	27)	(160	50)
(163	4)	(169	5)	(173	28)	(174	22)	(175	1000)
(176	169)	(177	78)	(178	6)	(184	4)	(188	6)
(189	13)	(190	15)	(199	5)	(200	20)	(203	12)
(204	8)	(205	44)	(211	5)	(215	11)	(216	7)
(218	14)	(219	7)	(221	15)	(230	10)	(231	102)
(232	19)	(233	6)	(234	11)	(235	10)	(245	5)
(250	6)	(259	6)	(264	10)	(265	21)	(266	5)
(283	4)	(284	6)	(287	4)	(288	5)	(289	5)
(290	5)	(291	9)	(292	9)	(297	6)	(299	7)
(306	6)	(316	7)	(317	6)	(320	6)	(321	20)
(324	24)	(325	6)	(334	6)	(335	5)	(369	4)
(370	6)	(380	4)	(381	5)	(382	18)	(383	6)
(389	5)	(396	5)	(397	9)	(418	5)	(424	5)
(436	6)	(443	4)	(452	5)	(456	5)	(481	5)
(495	5)	(534	6)	(544	4)	(548	5)		

NAME:13C\_1878.0\_1313EC11\_Fructose methoxyamine {BP} (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:188004-11-1

RI:1878

RT:11.688

NUM PEAKS: 68

( 70	5)	( 71	7)	( 72	20)	( 73	1000)	( 74	92)
( 75	79)	( 85	24)	( 86	13)	( 88	6)	( 89	55)
( 90	27)	( 91	4)	(101	9)	(102	9)	(103	50)
(104	222)	(105	34)	(106	9)	(114	3)	(115	7)
(116	21)	(117	10)	(118	19)	(119	59)	(120	8)
(129	3)	(130	3)	(131	24)	(132	70)	(133	76)
(135	12)	(145	8)	(146	14)	(147	217)	(148	52)
(164	3)	(175	3)	(176	11)	(177	8)	(178	3)
(190	4)	(191	32)	(192	24)	(193	6)	(203	7)
(204	6)	(208	17)	(219	11)	(220	172)	(221	40)
(222	18)	(235	7)	(236	3)	(248	6)	(249	3)
(262	4)	(265	8)	(266	5)	(279	10)	(280	4)
(294	3)	(308	3)	(309	5)	(310	40)	(311	11)

(312 5) (338 4) (368 6)

NAME:13C\_1824.4\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:182006-11-1

RI:1824

RT:11.274

NUM PEAKS: 205

( 76 309)	( 77 511)	( 78 165)	( 79 428)	( 81 43)
( 82 42)	( 83 61)	( 84 208)	( 91 135)	( 92 44)
( 93 247)	( 94 42)	( 95 133)	( 96 59)	( 97 112)
(107 30)	(108 23)	(109 22)	(110 35)	(111 51)
(112 42)	(120 31)	(121 32)	(124 13)	(125 41)
(126 58)	(127 78)	(137 24)	(140 38)	(141 87)
(142 52)	(152 37)	(153 27)	(154 25)	(155 57)
(156 34)	(165 30)	(169 62)	(170 124)	(182 23)
(184 117)	(195 28)	(196 48)	(197 73)	(198 118)
(199 35)	(200 20)	(210 49)	(212 106)	(214 31)
(224 27)	(225 25)	(226 26)	(227 27)	(228 29)
(240 27)	(241 33)	(242 49)	(243 36)	(244 22)
(245 43)	(254 35)	(255 23)	(256 26)	(268 25)
(269 204)	(270 1000)	(271 209)	(272 97)	(282 21)
(283 27)	(284 98)	(285 353)	(286 82)	(287 34)
(288 10)	(296 10)	(297 8)	(298 19)	(299 75)
(300 19)	(302 22)	(304 25)	(310 60)	(311 38)
(312 26)	(313 22)	(314 32)	(315 30)	(316 19)
(317 16)	(324 24)	(325 30)	(326 14)	(327 21)
(328 27)	(329 12)	(330 21)	(331 26)	(332 19)
(333 35)	(340 10)	(341 9)	(342 12)	(345 15)
(346 23)	(356 10)	(359 9)	(362 24)	(366 29)
(371 13)	(372 11)	(378 12)	(387 18)	(388 7)
(391 10)	(394 13)	(395 14)	(396 15)	(397 21)
(398 25)	(399 16)	(400 17)	(401 15)	(404 20)
(405 20)	(406 10)	(414 17)	(415 19)	(416 15)
(417 16)	(418 18)	(419 17)	(420 23)	(421 15)
(422 22)	(430 11)	(431 14)	(432 12)	(434 14)
(435 12)	(436 10)	(437 13)	(438 24)	(439 18)
(440 19)	(441 9)	(442 13)	(443 18)	(444 21)
(445 9)	(452 10)	(453 10)	(454 11)	(456 12)
(464 26)	(466 28)	(467 17)	(468 11)	(469 16)
(474 20)	(475 13)	(489 9)	(492 12)	(493 14)
(494 14)	(495 17)	(496 8)	(497 13)	(501 12)
(505 8)	(506 8)	(509 12)	(511 18)	(512 21)
(513 17)	(514 13)	(516 16)	(517 13)	(518 19)
(520 12)	(521 9)	(522 23)	(523 12)	(524 13)
(525 12)	(526 20)	(527 17)	(528 19)	(529 9)
(530 11)	(531 14)	(536 8)	(538 11)	(540 10)
(541 18)	(542 14)	(543 8)	(546 13)	(548 15)
(552 7)	(556 4)	(561 8)	(588 4)	(592 4)

NAME:13C\_1822.9\_1313EC11\_Citric acid (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:182004-11-1

RI:1823

RT:11.261

NUM PEAKS: 145

( 70 24)	( 71 111)	( 72 59)	( 73 1000)	( 74 10)
( 75 352)	( 76 22)	( 77 29)	( 78 3)	( 79 5)
( 83 4)	( 84 9)	( 85 24)	( 89 4)	( 93 12)
( 95 8)	( 96 5)	( 97 9)	( 98 5)	( 99 21)

(100	8)	(105	8)	(111	5)	(118	13)	(119	10)
(127	3)	(129	10)	(132	8)	(133	110)	(134	10)
(135	12)	(139	4)	(141	9)	(142	3)	(143	15)
(147	526)	(148	33)	(149	126)	(150	16)	(151	10)
(155	3)	(161	4)	(163	13)	(169	5)	(170	5)
(171	4)	(183	28)	(184	8)	(185	11)	(187	5)
(188	75)	(189	16)	(190	9)	(191	6)	(193	4)
(197	3)	(198	4)	(201	3)	(207	19)	(208	4)
(209	3)	(211	41)	(212	9)	(213	7)	(215	8)
(216	10)	(217	112)	(219	10)	(221	63)	(222	12)
(223	8)	(229	5)	(231	7)	(232	4)	(233	12)
(234	10)	(235	13)	(245	3)	(257	18)	(258	4)
(259	4)	(261	11)	(262	51)	(269	8)	(270	43)
(271	8)	(272	7)	(273	136)	(274	31)	(275	14)
(276	7)	(277	33)	(278	378)	(279	68)	(280	32)
(281	4)	(284	4)	(285	19)	(286	4)	(287	3)
(291	13)	(292	3)	(293	6)	(299	3)	(301	3)
(303	4)	(305	9)	(306	5)	(307	16)	(308	23)
(309	9)	(310	5)	(323	5)	(337	3)	(338	3)
(346	3)	(347	26)	(348	9)	(349	5)	(350	3)
(351	15)	(352	80)	(353	23)	(354	11)	(363	18)
(364	6)	(365	3)	(367	9)	(368	55)	(369	16)
(370	7)	(374	3)	(375	20)	(376	6)	(377	3)
(380	11)	(381	56)	(382	17)	(383	9)	(465	8)
(466	3)	(470	7)	(471	24)	(472	10)	(473	3)

NAME:13C\_1741.3\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:174003-11-1

RI:1741

RT:10.629

NUM PEAKS: 33

( 72	33)	( 73	1000)	( 74	59)	( 75	97)	( 76	13)
(101	106)	(108	11)	(113	16)	(116	14)	(117	22)
(129	19)	(130	21)	(131	44)	(133	48)	(143	17)
(147	280)	(148	42)	(149	22)	(163	99)	(173	82)
(174	20)	(184	10)	(204	48)	(205	44)	(207	215)
(208	29)	(221	14)	(231	48)	(281	17)	(291	9)
(292	21)	(307	29)	(410	12)				

NAME:13C\_1694.3\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:169001-11-1

RI:1694

RT:10.264

NUM PEAKS: 44

( 70	12)	( 73	1000)	( 74	53)	( 75	61)	( 90	60)
( 93	10)	(103	86)	(104	53)	(107	14)	(114	14)
(117	46)	(119	183)	(131	23)	(132	55)	(133	91)
(134	11)	(135	16)	(147	207)	(148	37)	(149	26)
(153	8)	(155	11)	(158	12)	(191	20)	(219	46)
(220	22)	(235	41)	(236	19)	(245	8)	(249	9)
(250	39)	(254	16)	(264	29)	(271	16)	(292	16)
(313	9)	(323	16)	(346	21)	(347	13)	(358	13)
(392	15)	(405	14)	(458	12)	(459	10)		

NAME:13C\_1673.0\_1313EC07\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:167003-11-1

RI:1673

RT:10.101

NUM PEAKS: 60

( 73 1000)	( 74 100)	( 75 212)	( 76 15)	( 85 14)
( 86 50)	( 87 123)	( 98 3)	( 99 8)	(100 11)
(102 55)	(103 476)	(112 4)	(115 29)	(117 17)
(118 27)	(127 3)	(142 3)	(144 7)	(158 11)
(159 7)	(160 39)	(161 26)	(172 3)	(175 51)
(176 28)	(184 2)	(186 3)	(187 2)	(188 4)
(189 18)	(200 2)	(201 2)	(204 5)	(214 2)
(215 2)	(229 2)	(230 2)	(248 11)	(249 9)
(250 5)	(277 3)	(292 6)	(293 69)	(294 500)
(295 99)	(296 43)	(297 5)	(321 2)	(322 8)
(323 3)	(350 2)	(351 10)	(352 4)	(353 3)
(368 13)	(369 5)	(370 2)	(396 2)	(397 2)

NAME:13C\_1562.0\_1313EC11\_Cysteine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:156002-11-1

RI:1562

RT:9.232

NUM PEAKS: 115

( 70 174)	( 71 121)	( 72 45)	( 73 1000)	( 74 199)
( 75 502)	( 76 45)	( 77 24)	( 80 9)	( 81 9)
( 82 17)	( 83 124)	( 85 100)	( 86 14)	( 87 44)
( 88 37)	( 89 41)	( 90 9)	( 91 49)	( 92 8)
( 94 5)	( 95 5)	( 96 35)	( 97 41)	( 98 351)
( 99 49)	(100 68)	(101 60)	(102 39)	(103 30)
(104 55)	(105 4)	(106 6)	(110 24)	(111 140)
(112 13)	(113 17)	(114 9)	(115 13)	(116 8)
(117 23)	(118 35)	(119 31)	(120 6)	(121 4)
(123 3)	(124 6)	(125 23)	(126 63)	(127 144)
(130 5)	(131 23)	(132 250)	(133 72)	(134 26)
(135 5)	(137 3)	(139 26)	(140 8)	(141 9)
(143 12)	(145 6)	(146 5)	(147 130)	(153 5)
(154 5)	(155 9)	(156 13)	(157 6)	(158 6)
(159 67)	(161 12)	(163 8)	(168 9)	(169 10)
(172 6)	(173 9)	(174 4)	(175 14)	(177 5)
(183 6)	(184 15)	(185 21)	(187 4)	(200 3)
(201 4)	(202 18)	(206 8)	(208 4)	(212 4)
(213 42)	(214 8)	(218 5)	(219 5)	(220 76)
(221 19)	(222 81)	(223 13)	(224 10)	(230 5)
(231 30)	(232 4)	(235 5)	(236 3)	(237 8)
(244 4)	(250 3)	(251 9)	(252 4)	(264 4)
(265 3)	(279 3)	(285 5)	(286 3)	(296 4)

NAME:13C\_1279.2\_1313EC16\_Serine (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:128001-11-1

RI:1279

RT:6.160

NUM PEAKS: 40

( 72 20)	( 73 1000)	( 74 114)	( 75 320)	( 76 27)
( 77 9)	( 81 44)	( 86 7)	( 87 86)	( 88 32)
( 89 41)	( 90 9)	( 91 7)	(101 40)	(102 91)
(103 27)	(104 112)	(105 8)	(116 28)	(117 39)
(118 652)	(119 67)	(120 20)	(130 5)	(131 14)
(132 60)	(133 82)	(134 446)	(135 36)	(136 12)
(145 6)	(147 89)	(148 54)	(149 12)	(162 30)
(174 5)	(208 5)	(221 20)	(228 7)	(237 17)



NAME:13C\_1220.5\_1313EC11\_Valine (2TMS)  
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
 CASNO:122001-11-1

RI:1221

RT:5.509

NUM PEAKS: 25

( 70	12)	( 72	35)	( 73	981)	( 74	127)	( 75	355)
( 76	99)	( 79	48)	( 87	43)	( 88	19)	(100	21)
(101	112)	(102	28)	(103	16)	(104	13)	(117	35)
(131	23)	(132	66)	(133	58)	(147	192)	(148	1000)
(149	100)	(150	39)	(161	15)	(220	75)	(222	41)

NAME:13C\_1314.0\_1313EC16\_Isoleucine (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:132002-11-1

RI:1314

RT:6.570

NUM PEAKS: 27

( 90	6)	( 91	25)	(101	80)	(118	8)	(132	49)
(158	10)	(160	9)	(161	9)	(162	47)	(163	1000)
(164	88)	(165	30)	(196	1)	(203	1)	(204	2)
(205	6)	(207	5)	(215	1)	(220	52)	(236	2)
(237	37)	(238	9)	(239	3)	(266	8)	(267	2)
(268	1)	(347	1)						

NAME:13C\_1354.8\_1313EC11\_Glyceric acid (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:135003-11-1

RI:1355

RT:7.049

NUM PEAKS: 14

( 73	1000)	( 74	82)	(103	176)	(104	107)	(118	23)
(119	71)	(131	35)	(132	50)	(133	190)	(147	359)
(148	57)	(191	224)	(207	37)	(294	62)		

NAME:13C\_1372.0\_1313EC11\_Fumaric acid (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:137001-11-1

RI:1372

RT:7.282

NUM PEAKS: 124

( 70	21)	( 71	81)	( 72	7)	( 73	1000)	( 74	112)
( 75	527)	( 76	32)	( 80	9)	( 81	21)	( 82	27)
( 83	114)	( 84	43)	( 85	152)	( 86	42)	( 94	12)
( 95	11)	( 97	17)	( 98	5)	(101	15)	(103	9)
(104	3)	(105	14)	(106	4)	(108	10)	(109	8)
(110	16)	(111	7)	(112	17)	(113	5)	(114	6)
(115	68)	(116	21)	(117	56)	(118	9)	(119	4)
(124	7)	(127	27)	(128	13)	(129	24)	(130	19)
(131	28)	(132	8)	(133	137)	(134	25)	(135	16)
(136	4)	(139	10)	(141	4)	(142	6)	(143	111)
(144	25)	(145	22)	(146	90)	(147	792)	(148	127)
(149	90)	(150	17)	(151	4)	(152	14)	(155	43)
(156	24)	(157	40)	(158	15)	(159	56)	(160	1)
(165	3)	(167	3)	(170	4)	(171	41)	(172	16)
(176	1)	(177	12)	(178	6)	(180	2)	(185	1)
(186	2)	(188	3)	(190	3)	(191	12)	(192	7)
(193	2)	(195	9)	(198	1)	(199	12)	(200	3)
(202	8)	(206	1)	(209	4)	(210	6)	(214	2)
(216	2)	(217	22)	(218	11)	(219	5)	(220	15)

(221	8)	(225	7)	(228	3)	(229	2)	(230	4)
(231	3)	(232	1)	(234	6)	(238	3)	(240	6)
(244	12)	(245	437)	(246	91)	(247	32)	(248	28)
(249	324)	(250	48)	(251	15)	(253	2)	(254	6)
(259	2)	(260	4)	(264	1)	(265	3)	(269	10)
(270	6)	(271	12)	(272	2)	(273	2)		

NAME:13C\_1449.3\_1313EC16\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:144007-11-1

RI:1449

RT:8.163

NUM PEAKS: 308

( 72	69)	( 73	1000)	( 74	220)	( 75	423)	( 76	73)
( 77	47)	( 79	38)	( 82	2)	( 83	12)	( 84	4)
( 85	17)	( 86	16)	( 87	9)	( 88	15)	( 89	27)
( 90	16)	( 91	12)	( 92	25)	( 93	9)	( 94	8)
( 97	6)	( 98	19)	(100	19)	(101	47)	(102	65)
(103	41)	(104	50)	(105	18)	(109	14)	(110	7)
(111	10)	(112	11)	(115	32)	(116	11)	(117	23)
(118	202)	(119	154)	(120	14)	(121	21)	(122	16)
(126	3)	(128	8)	(129	5)	(130	14)	(131	23)
(132	207)	(133	73)	(134	9)	(135	12)	(137	11)
(138	12)	(139	1)	(140	15)	(142	32)	(143	4)
(146	21)	(147	328)	(148	57)	(149	35)	(151	8)
(152	2)	(155	10)	(156	29)	(158	15)	(159	15)
(160	15)	(162	27)	(163	327)	(164	27)	(165	10)
(167	2)	(168	5)	(169	3)	(171	1)	(174	6)
(175	22)	(176	14)	(177	2)	(179	4)	(180	10)
(181	7)	(182	11)	(184	9)	(186	27)	(187	9)
(190	2)	(192	1)	(193	12)	(195	15)	(196	5)
(197	17)	(200	27)	(201	3)	(202	22)	(204	13)
(205	25)	(206	1)	(207	9)	(212	8)	(214	8)
(216	6)	(223	6)	(226	18)	(229	7)	(232	5)
(234	13)	(235	13)	(236	25)	(237	17)	(238	1)
(241	2)	(242	5)	(246	4)	(249	42)	(250	1)
(252	17)	(255	11)	(256	2)	(257	19)	(258	27)
(259	2)	(266	12)	(269	5)	(272	6)	(276	19)
(277	3)	(278	9)	(281	1)	(283	24)	(284	8)
(288	6)	(289	2)	(290	7)	(294	7)	(295	3)
(298	4)	(312	13)	(313	1)	(314	7)	(315	1)
(321	5)	(322	4)	(326	7)	(327	18)	(328	7)
(329	6)	(330	2)	(333	7)	(334	18)	(335	17)
(336	8)	(337	3)	(338	4)	(342	18)	(344	9)
(345	18)	(346	5)	(349	13)	(350	5)	(352	6)
(353	7)	(354	12)	(356	20)	(357	11)	(358	21)
(361	15)	(362	14)	(363	6)	(365	8)	(366	19)
(367	9)	(368	18)	(370	1)	(371	2)	(372	5)
(373	11)	(375	16)	(379	6)	(380	6)	(381	22)
(382	2)	(383	18)	(384	8)	(386	11)	(387	3)
(388	7)	(389	18)	(390	10)	(393	8)	(394	6)
(396	10)	(397	8)	(400	22)	(401	2)	(402	18)
(404	11)	(405	10)	(406	4)	(407	7)	(409	11)
(410	1)	(413	1)	(414	21)	(415	5)	(416	26)
(417	13)	(419	2)	(422	5)	(424	9)	(425	1)
(426	15)	(429	10)	(431	12)	(432	8)	(433	10)
(436	13)	(438	23)	(441	8)	(444	27)	(445	8)
(447	3)	(448	6)	(449	12)	(452	18)	(453	15)
(454	11)	(457	13)	(459	4)	(460	24)	(461	16)
(462	1)	(464	8)	(466	18)	(467	5)	(471	12)

(472	15)	(475	31)	(476	3)	(477	1)	(481	10)
(482	13)	(483	2)	(486	2)	(487	3)	(488	14)
(489	29)	(490	21)	(492	1)	(493	3)	(494	18)
(496	3)	(499	17)	(500	7)	(502	6)	(503	3)
(506	24)	(507	9)	(508	1)	(509	28)	(511	12)
(512	6)	(513	3)	(517	11)	(518	14)	(519	1)
(523	12)	(525	14)	(527	12)	(530	23)	(531	19)
(533	4)	(534	14)	(535	2)	(537	9)	(538	6)
(539	4)	(541	15)	(542	5)	(548	12)	(553	13)
(554	5)	(559	3)	(560	4)	(563	14)	(564	3)
(565	7)	(568	2)	(569	11)	(571	11)	(573	3)
(574	4)	(575	12)	(576	4)	(578	4)	(579	4)
(580	5)	(582	6)	(583	9)	(584	1)	(585	1)
(586	1)	(587	6)	(591	1)	(592	17)	(593	4)
(595	3)	(596	3)	(597	1)				

NAME:13C\_1726.4\_1313EC11\_Fucose methoxyamine (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:173002-11-1

RI:1726

RT:10.512

NUM PEAKS: 37

( 72	106)	( 73	999)	(103	153)	(106	69)	(116	32)
(117	68)	(118	45)	(119	1000)	(120	73)	(131	164)
(134	51)	(135	40)	(137	33)	(146	50)	(148	204)
(149	120)	(175	25)	(190	63)	(191	164)	(192	128)
(193	40)	(205	27)	(219	34)	(222	65)	(235	26)
(249	25)	(250	123)	(260	14)	(294	32)	(309	19)
(311	36)	(322	52)	(324	40)	(337	33)	(398	20)
(500	17)	(537	15)						

NAME:13C\_1785.2\_1313EC07\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:179001-11-1

RI:1785

RT:10.978

NUM PEAKS: 337

( 72	18)	( 73	1000)	( 74	72)	( 75	49)	( 76	9)
( 78	3)	( 82	3)	( 86	3)	( 88	3)	( 89	5)
( 90	18)	( 91	12)	( 92	2)	( 94	2)	( 96	1)
( 97	2)	(103	52)	(104	225)	(105	24)	(106	9)
(107	2)	(108	2)	(109	2)	(115	8)	(117	3)
(118	9)	(119	58)	(120	6)	(121	4)	(122	2)
(128	1)	(129	3)	(131	21)	(132	63)	(133	93)
(134	29)	(135	13)	(138	2)	(140	2)	(141	1)
(144	2)	(145	9)	(146	29)	(147	213)	(148	42)
(149	34)	(150	7)	(151	4)	(152	1)	(154	1)
(155	3)	(157	1)	(159	2)	(161	10)	(162	3)
(163	2)	(164	3)	(165	4)	(166	1)	(167	3)
(168	2)	(176	3)	(177	8)	(178	3)	(179	4)
(180	3)	(181	6)	(182	2)	(183	2)	(184	2)
(187	1)	(188	2)	(189	4)	(191	47)	(192	22)
(193	9)	(195	7)	(196	1)	(197	2)	(199	2)
(200	2)	(202	1)	(205	4)	(206	51)	(207	41)
(208	9)	(209	4)	(210	4)	(211	12)	(213	3)
(214	2)	(215	1)	(216	1)	(217	2)	(218	2)
(219	5)	(220	131)	(221	42)	(222	15)	(223	3)
(224	1)	(228	3)	(231	1)	(233	3)	(234	3)
(238	1)	(239	2)	(240	1)	(242	3)	(243	3)
(244	2)	(245	2)	(246	1)	(247	1)	(248	1)

(249	3)	(252	2)	(253	2)	(254	2)	(256	3)
(257	2)	(259	3)	(261	1)	(262	9)	(263	4)
(264	5)	(266	3)	(269	2)	(272	1)	(273	1)
(274	2)	(275	2)	(276	2)	(277	2)	(279	14)
(280	5)	(281	1)	(282	2)	(284	1)	(285	4)
(286	2)	(287	2)	(288	1)	(291	1)	(292	3)
(293	11)	(294	137)	(295	38)	(296	18)	(297	3)
(298	4)	(299	6)	(300	4)	(301	4)	(302	2)
(303	1)	(305	1)	(306	1)	(307	5)	(308	20)
(309	8)	(310	19)	(311	5)	(312	3)	(315	3)
(316	2)	(317	2)	(318	2)	(319	2)	(320	1)
(322	1)	(323	3)	(324	3)	(330	2)	(332	3)
(333	2)	(335	3)	(336	10)	(337	15)	(338	6)
(339	3)	(340	2)	(343	1)	(345	2)	(346	2)
(348	2)	(349	3)	(351	6)	(352	5)	(353	3)
(354	1)	(358	2)	(360	2)	(362	2)	(363	2)
(364	2)	(365	1)	(366	2)	(369	2)	(370	1)
(372	3)	(373	4)	(374	3)	(375	2)	(382	3)
(383	2)	(384	2)	(386	2)	(387	3)	(389	2)
(390	3)	(391	2)	(392	2)	(394	2)	(396	2)
(397	2)	(398	1)	(399	2)	(400	1)	(404	2)
(405	2)	(406	2)	(408	2)	(410	1)	(411	1)
(412	1)	(416	2)	(420	1)	(421	2)	(422	2)
(423	2)	(424	3)	(425	2)	(426	5)	(427	3)
(428	1)	(432	2)	(433	2)	(434	2)	(435	3)
(436	2)	(438	2)	(439	2)	(440	1)	(441	2)
(442	2)	(444	2)	(445	3)	(446	2)	(447	2)
(448	3)	(449	2)	(450	2)	(451	1)	(452	2)
(453	2)	(454	2)	(455	1)	(456	2)	(457	2)
(458	1)	(459	1)	(460	2)	(461	2)	(462	2)
(463	2)	(464	2)	(465	3)	(467	1)	(468	1)
(469	1)	(470	2)	(472	2)	(473	2)	(474	2)
(475	1)	(478	2)	(480	2)	(481	2)	(483	2)
(485	2)	(486	2)	(487	2)	(488	2)	(489	1)
(490	2)	(491	2)	(492	1)	(496	1)	(497	1)
(498	2)	(499	2)	(500	2)	(502	2)	(503	1)
(504	2)	(506	1)	(508	2)	(510	1)	(511	2)
(512	2)	(513	1)	(514	2)	(515	3)	(516	4)
(517	3)	(518	2)	(519	2)	(520	2)	(521	1)
(522	2)	(523	2)	(525	3)	(526	2)	(527	2)
(530	2)	(531	1)	(533	2)	(534	2)	(535	2)
(539	2)	(540	2)	(541	3)	(544	1)	(545	2)
(546	1)	(548	1)	(552	2)	(555	1)	(556	1)
(559	1)	(564	1)	(570	1)	(571	1)	(572	1)
(573	1)	(575	1)						

NAME:13C\_1802.7\_1313EC07

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:180002-11-1

RI:1803

RT:11.114

NUM PEAKS: 85

( 72	9)	( 73	1000)	( 74	103)	( 75	108)	( 76	12)
( 87	5)	( 90	8)	( 92	1)	( 94	1)	(102	4)
(103	21)	(104	13)	(114	5)	(116	2)	(118	9)
(119	25)	(130	1)	(131	27)	(132	46)	(133	32)
(134	6)	(135	7)	(136	1)	(140	4)	(144	2)
(145	26)	(146	21)	(147	102)	(148	15)	(149	11)
(157	2)	(159	1)	(161	19)	(174	9)	(177	1)
(186	1)	(188	2)	(189	2)	(190	1)	(191	15)

(192	35)	(193	8)	(194	3)	(207	9)	(208	2)
(218	2)	(219	10)	(220	34)	(221	24)	(233	6)
(234	3)	(242	1)	(248	2)	(249	1)	(250	3)
(251	4)	(252	1)	(260	1)	(261	2)	(262	49)
(263	6)	(264	3)	(278	6)	(279	4)	(292	1)
(294	3)	(295	12)	(296	1)	(297	1)	(307	6)
(308	1)	(323	6)	(324	1)	(352	5)	(353	2)
(354	2)	(368	2)	(369	1)	(429	1)	(441	7)
(442	30)	(443	14)	(444	5)	(512	1)	(564	1)

NAME:13C\_1805.7\_1313EC07

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:181004-11-1

RI:1806

RT:11.136

NUM PEAKS: 125

( 70	10)	( 71	8)	( 72	12)	( 73	1000)	( 74	100)
( 75	144)	( 76	13)	( 77	8)	( 81	3)	( 82	5)
( 83	16)	( 84	5)	( 85	5)	( 86	11)	( 87	5)
( 90	10)	( 91	5)	( 92	1)	( 93	1)	( 94	1)
( 95	2)	( 96	3)	( 97	15)	( 98	3)	(100	2)
(101	3)	(102	4)	(103	17)	(104	28)	(109	1)
(110	1)	(111	7)	(112	2)	(114	6)	(115	3)
(116	5)	(117	5)	(118	10)	(119	41)	(120	3)
(121	1)	(124	2)	(125	3)	(129	7)	(130	2)
(131	22)	(132	50)	(133	34)	(134	7)	(135	6)
(136	1)	(140	5)	(141	1)	(144	3)	(145	27)
(146	15)	(147	110)	(148	18)	(149	22)	(150	2)
(151	1)	(152	2)	(153	1)	(154	1)	(159	1)
(160	4)	(161	19)	(174	15)	(176	2)	(179	1)
(188	3)	(189	2)	(190	2)	(191	13)	(196	2)
(201	2)	(204	3)	(214	1)	(217	2)	(218	5)
(219	15)	(220	98)	(221	34)	(222	8)	(223	2)
(224	1)	(233	7)	(234	6)	(237	1)	(248	3)
(249	1)	(251	3)	(260	1)	(261	4)	(262	56)
(263	8)	(264	5)	(265	2)	(276	1)	(278	4)
(279	4)	(280	1)	(294	2)	(295	8)	(296	2)
(307	8)	(308	3)	(309	1)	(317	2)	(323	7)
(324	2)	(336	1)	(351	1)	(352	7)	(353	2)
(354	2)	(368	3)	(369	1)	(370	1)	(440	1)
(441	10)	(442	40)	(443	17)	(444	8)	(445	1)

NAME:13C\_1842.0\_1313EC11

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:184002-11-1

RI:1842

RT:11.427

NUM PEAKS: 140

( 70	11)	( 71	8)	( 72	30)	( 73	1000)	( 74	101)
( 75	178)	( 76	10)	( 77	17)	( 78	3)	( 79	4)
( 85	75)	( 86	6)	( 87	19)	( 88	5)	( 89	6)
( 90	15)	( 91	3)	( 92	1)	( 93	4)	( 94	1)
( 95	3)	( 97	1)	( 98	6)	( 99	25)	(100	23)
(101	28)	(102	16)	(103	55)	(104	44)	(105	9)
(106	2)	(113	3)	(114	9)	(115	13)	(116	8)
(117	15)	(118	16)	(119	72)	(120	5)	(121	1)
(127	1)	(129	10)	(130	10)	(131	23)	(133	56)
(134	12)	(135	4)	(141	11)	(142	6)	(143	8)
(144	5)	(145	16)	(146	13)	(147	171)	(148	29)
(157	31)	(158	28)	(159	10)	(160	4)	(161	7)

(162	14)	(163	1)	(170	4)	(171	19)	(172	72)
(173	526)	(174	227)	(175	32)	(176	6)	(177	6)
(178	2)	(179	1)	(185	3)	(186	3)	(187	7)
(188	2)	(189	2)	(190	2)	(191	5)	(192	15)
(193	3)	(198	1)	(199	1)	(200	1)	(201	13)
(202	3)	(203	2)	(204	1)	(209	1)	(211	1)
(212	1)	(213	5)	(214	1)	(215	2)	(216	1)
(217	1)	(219	2)	(220	19)	(221	5)	(222	3)
(231	2)	(232	2)	(243	6)	(244	9)	(245	25)
(246	29)	(247	8)	(248	1)	(260	3)	(261	5)
(262	23)	(263	5)	(264	1)	(266	3)	(270	3)
(273	1)	(274	1)	(275	8)	(276	3)	(285	1)
(289	1)	(290	13)	(291	3)	(307	3)	(308	1)
(334	6)	(335	2)	(336	2)	(337	1)	(352	2)
(353	1)	(365	5)	(366	1)	(374	1)	(380	9)
(381	2)	(441	3)	(442	15)	(443	6)	(444	1)

NAME:13C\_1847.4\_1313EC07

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:185003-11-1

RI:1847

RT:11.461

NUM PEAKS: 205

( 71	111)	( 74	923)	( 75	999)	( 76	60)	( 77	33)
( 80	5)	( 86	69)	( 87	109)	( 88	35)	( 89	133)
( 90	149)	( 91	23)	( 92	9)	( 94	6)	( 96	11)
(101	170)	(102	109)	(104	542)	(105	78)	(106	25)
(108	5)	(112	16)	(115	158)	(116	59)	(118	157)
(120	49)	(121	25)	(130	87)	(131	346)	(132	605)
(134	142)	(135	76)	(136	10)	(138	6)	(139	5)
(144	76)	(146	151)	(150	38)	(151	22)	(153	4)
(155	15)	(159	84)	(160	1000)	(161	714)	(162	190)
(163	178)	(164	33)	(165	11)	(166	5)	(167	3)
(168	4)	(178	44)	(179	14)	(184	7)	(188	14)
(189	37)	(190	27)	(191	374)	(196	3)	(197	7)
(198	11)	(203	40)	(204	47)	(205	61)	(207	249)
(209	23)	(210	4)	(212	8)	(215	10)	(217	22)
(218	40)	(223	30)	(224	8)	(226	4)	(229	7)
(230	13)	(232	73)	(233	49)	(234	99)	(235	97)
(236	35)	(237	22)	(238	9)	(239	4)	(248	150)
(249	72)	(250	32)	(251	60)	(252	12)	(253	7)
(254	4)	(256	3)	(261	12)	(263	18)	(269	8)
(271	4)	(272	5)	(274	14)	(277	58)	(278	29)
(280	10)	(281	10)	(282	5)	(289	13)	(292	10)
(294	35)	(295	12)	(296	5)	(297	3)	(298	5)
(306	16)	(307	22)	(319	5)	(321	21)	(322	271)
(323	212)	(324	81)	(325	22)	(326	8)	(331	5)
(335	20)	(338	14)	(339	6)	(340	4)	(341	6)
(342	5)	(343	4)	(346	5)	(347	6)	(348	5)
(349	7)	(350	11)	(351	55)	(352	46)	(353	22)
(354	11)	(359	4)	(362	6)	(363	3)	(368	11)
(369	6)	(372	6)	(377	4)	(383	5)	(384	5)
(387	4)	(388	5)	(391	5)	(396	8)	(397	8)
(398	8)	(404	3)	(405	6)	(410	3)	(412	9)
(413	5)	(416	4)	(424	7)	(425	33)	(426	13)
(427	6)	(431	3)	(434	3)	(438	5)	(439	6)
(440	4)	(441	10)	(444	10)	(447	6)	(448	5)
(454	4)	(455	3)	(459	4)	(461	5)	(462	5)
(463	4)	(466	7)	(467	5)	(469	4)	(470	4)
(477	5)	(489	3)	(492	2)	(496	5)	(499	3)

97

(504	4)	(521	3)	(527	4)	(538	2)	(541	3)
(542	4)	(545	3)	(551	2)	(553	3)	(556	2)
(559	2)	(560	3)	(563	3)	(567	2)	(569	4)
(570	2)	(572	4)	(573	2)	(588	3)	(590	2)

NAME:13C\_1869.1\_1313EC11\_Fructose methoxyamine (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:187002-11-1

RI:1869

RT:11.620

NUM PEAKS: 110

( 72	19)	( 73	1000)	( 74	96)	( 76	3)	( 85	19)
( 86	5)	( 88	5)	( 89	19)	( 90	19)	( 91	3)
( 92	1)	(102	6)	(103	35)	(104	174)	(105	20)
(106	7)	(107	1)	(116	9)	(117	9)	(118	7)
(119	50)	(120	5)	(121	2)	(131	26)	(132	25)
(133	55)	(134	23)	(135	8)	(136	1)	(145	7)
(146	7)	(147	206)	(148	38)	(149	23)	(150	2)
(151	1)	(160	4)	(161	5)	(163	4)	(164	2)
(165	1)	(175	2)	(176	9)	(177	8)	(178	4)
(179	1)	(188	2)	(190	2)	(191	15)	(192	8)
(193	3)	(194	1)	(203	6)	(204	3)	(205	3)
(206	16)	(207	18)	(208	5)	(209	2)	(210	1)
(217	4)	(218	2)	(219	5)	(220	80)	(221	17)
(222	8)	(223	1)	(233	2)	(234	2)	(235	1)
(236	1)	(237	1)	(249	1)	(250	1)	(261	2)
(262	1)	(263	1)	(264	1)	(265	2)	(266	3)
(267	1)	(268	1)	(277	1)	(278	1)	(279	7)
(280	3)	(281	2)	(282	1)	(291	1)	(293	1)
(294	2)	(295	1)	(296	1)	(305	1)	(306	1)
(307	1)	(308	1)	(309	2)	(310	28)	(311	7)
(312	3)	(335	1)	(337	1)	(338	2)	(339	1)
(354	1)	(367	1)	(368	4)	(369	2)	(370	1)

NAME:13C\_2137.1\_1313EC16

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:214003-11-1

RI:2137

RT:13.366

NUM PEAKS: 65

( 72	12)	( 73	1000)	( 74	81)	( 75	68)	( 85	12)
( 86	11)	( 87	15)	( 89	32)	( 90	19)	( 99	6)
(101	4)	(102	10)	(103	21)	(104	181)	(105	15)
(106	7)	(116	15)	(117	10)	(118	10)	(119	67)
(120	4)	(131	25)	(132	77)	(133	50)	(134	46)
(135	7)	(145	4)	(146	12)	(147	244)	(148	35)
(149	18)	(151	5)	(158	6)	(161	67)	(162	7)
(169	3)	(173	19)	(174	5)	(176	8)	(177	8)
(191	25)	(192	11)	(203	6)	(204	5)	(206	28)
(207	120)	(208	20)	(220	74)	(233	14)	(235	8)
(236	3)	(250	4)	(265	6)	(274	3)	(279	7)
(308	4)	(322	12)	(323	118)	(324	35)	(325	14)
(422	4)	(449	3)	(466	5)	(478	3)	(590	3)

NAME:13C\_2246.0\_1313EC16-Octadecanoic acid (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:225002-11-1

RI:2246

RT:14.010

NUM PEAKS: 87

( 72	70)	( 75	1000)	( 76	106)	( 77	52)	( 78	7)
( 88	25)	( 89	82)	( 90	9)	( 91	31)	( 92	9)
( 93	17)	( 94	3)	(106	20)	(107	10)	(118	135)
(119	540)	(120	41)	(121	30)	(125	3)	(128	7)
(132	504)	(134	364)	(135	69)	(136	17)	(146	22)
(148	153)	(149	31)	(151	6)	(158	4)	(160	7)
(162	12)	(163	23)	(170	3)	(178	3)	(187	12)
(192	20)	(194	4)	(205	3)	(208	35)	(214	4)
(219	4)	(220	12)	(223	9)	(233	4)	(234	5)
(235	5)	(237	6)	(246	5)	(252	7)	(253	8)
(254	3)	(260	3)	(265	4)	(268	13)	(269	3)
(279	3)	(284	3)	(308	3)	(313	6)	(314	7)
(319	4)	(323	4)	(328	6)	(334	3)	(337	4)
(357	15)	(358	28)	(359	97)	(360	19)	(367	3)
(374	18)	(395	3)	(400	5)	(421	4)	(427	3)
(434	3)	(436	3)	(443	3)	(444	5)	(467	4)
(488	3)	(491	4)	(499	5)	(506	4)	(507	4)
(520	3)	(535	3)						

NAME:13C\_2327.6\_1313EC16\_Glucose-6-phosphate methoxyamine (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:233002-11-1

RI:2328

RT:14.442

NUM PEAKS: 51

( 72	20)	( 73	1000)	( 74	79)	( 75	77)	( 80	17)
( 87	19)	( 89	36)	(101	18)	(103	46)	(104	30)
(105	39)	(116	21)	(118	25)	(119	18)	(131	30)
(132	72)	(133	77)	(134	24)	(135	29)	(142	10)
(146	20)	(147	150)	(148	24)	(161	50)	(162	85)
(175	12)	(191	14)	(193	18)	(206	17)	(207	20)
(211	37)	(220	32)	(225	20)	(260	7)	(275	9)
(278	14)	(283	12)	(299	100)	(300	30)	(314	15)
(315	41)	(317	12)	(332	13)	(359	36)	(360	18)
(386	32)	(387	113)	(388	46)	(389	25)	(476	10)
(541	11)								

NAME:13C\_2748.0\_1313EC16\_Trehalose (8TMS); alpha-D-Glc-(1,1)-alpha-D-Glc

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:274002-11-1

RI:2748

RT:16.667

NUM PEAKS: 110

( 71	5)	( 72	15)	( 73	1000)	( 74	83)	( 85	5)
( 86	23)	( 87	11)	( 88	4)	( 89	6)	( 90	13)
(100	3)	(101	7)	(102	9)	(103	22)	(104	181)
(105	19)	(106	7)	(114	4)	(115	17)	(116	11)
(117	8)	(118	16)	(119	58)	(120	6)	(130	4)
(131	24)	(132	151)	(133	72)	(134	16)	(135	7)
(144	6)	(145	8)	(146	23)	(147	268)	(148	48)
(149	34)	(150	4)	(158	6)	(159	5)	(160	31)
(161	26)	(162	5)	(163	4)	(164	4)	(173	6)
(174	103)	(175	15)	(176	12)	(177	10)	(178	6)
(189	10)	(190	4)	(191	42)	(192	254)	(193	46)
(194	21)	(204	3)	(205	10)	(206	92)	(207	34)
(208	12)	(209	3)	(218	5)	(219	8)	(220	148)
(221	48)	(222	20)	(223	5)	(232	4)	(233	12)
(234	9)	(235	14)	(236	10)	(237	4)	(246	5)
(247	5)	(248	52)	(249	18)	(250	9)	(251	4)
(261	3)	(262	6)	(263	3)	(264	5)	(266	4)



(267	5)	(276	4)	(277	48)	(278	10)	(279	10)
(280	5)	(293	5)	(294	13)	(295	5)	(308	11)
(309	5)	(310	3)	(322	6)	(323	17)	(324	7)
(325	3)	(336	15)	(337	9)	(338	4)	(366	27)
(367	211)	(368	69)	(369	33)	(370	7)	(441	3)

NAME:13C\_3269.3\_1313EC16\_Ergosterol (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:327001-11-1

RI:3269

RT:19.000

NUM PEAKS: 216

( 70	52)	( 71	91)	( 72	223)	( 73	1000)	( 74	477)
( 75	395)	( 76	47)	( 77	13)	( 80	16)	( 81	15)
( 82	35)	( 83	92)	( 84	49)	( 85	151)	( 86	68)
( 87	273)	( 88	97)	( 89	98)	( 90	9)	( 91	12)
( 92	5)	( 93	7)	( 94	9)	( 95	8)	( 96	28)
( 97	32)	( 98	180)	( 99	31)	(100	117)	(101	39)
(102	105)	(103	45)	(104	27)	(105	5)	(106	5)
(107	3)	(109	6)	(110	13)	(111	24)	(112	28)
(113	137)	(114	23)	(115	78)	(116	34)	(117	61)
(118	34)	(119	12)	(120	3)	(122	6)	(123	15)
(124	99)	(125	30)	(126	89)	(127	43)	(128	195)
(129	14)	(130	32)	(131	21)	(132	94)	(133	82)
(134	168)	(135	18)	(136	21)	(137	59)	(138	166)
(139	132)	(140	42)	(141	123)	(142	22)	(143	51)
(144	11)	(145	22)	(146	12)	(147	23)	(148	112)
(149	15)	(150	20)	(151	30)	(152	159)	(153	114)
(154	271)	(155	58)	(156	161)	(157	20)	(158	42)
(159	9)	(160	26)	(161	7)	(162	10)	(163	16)
(164	43)	(165	59)	(166	51)	(167	133)	(168	76)
(169	241)	(170	70)	(171	133)	(172	12)	(173	13)
(174	16)	(175	37)	(176	12)	(177	17)	(178	57)
(179	30)	(180	55)	(181	44)	(182	111)	(183	46)
(184	95)	(185	17)	(186	24)	(187	6)	(188	8)
(189	13)	(190	7)	(191	8)	(192	21)	(193	26)
(194	23)	(195	57)	(196	40)	(197	102)	(198	31)
(199	74)	(200	11)	(201	12)	(202	9)	(203	6)
(204	10)	(205	5)	(206	7)	(207	7)	(209	21)
(211	40)	(212	102)	(213	32)	(214	63)	(215	7)
(216	13)	(217	3)	(218	4)	(219	5)	(220	4)
(221	4)	(222	4)	(223	10)	(224	14)	(225	46)
(226	42)	(227	138)	(228	24)	(229	46)	(230	4)
(231	3)	(232	8)	(233	3)	(237	3)	(238	8)
(239	10)	(240	26)	(241	17)	(242	34)	(243	32)
(244	20)	(245	4)	(256	18)	(257	30)	(258	5)
(259	3)	(268	7)	(269	14)	(270	49)	(271	34)
(272	93)	(273	5)	(284	5)	(285	14)	(286	6)
(287	7)	(298	3)	(299	4)	(300	9)	(301	7)
(302	3)	(304	3)	(314	5)	(315	8)	(316	3)
(330	3)	(332	3)	(346	4)	(347	3)	(348	3)
(349	5)	(358	5)	(359	18)	(360	40)	(361	104)
(362	52)	(363	8)	(386	7)	(387	24)	(388	58)
(389	146)	(390	68)	(391	9)	(403	8)	(404	19)
(405	38)	(406	18)	(494	13)	(495	27)	(496	16)
(497	4)								

NAME:13C\_2109.4\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:211004-11-1

100

RI:2109

RT:13.190

NUM PEAKS: 70

( 72	29)	( 73	1000)	( 74	86)	( 75	98)	( 77	12)
( 89	46)	( 90	11)	( 99	6)	(102	16)	(103	59)
(105	25)	(115	14)	(116	17)	(117	15)	(118	20)
(119	22)	(130	9)	(131	33)	(132	122)	(133	81)
(134	20)	(135	19)	(137	8)	(146	11)	(147	158)
(148	29)	(149	21)	(151	8)	(157	4)	(161	34)
(162	45)	(163	16)	(164	6)	(165	4)	(173	12)
(177	7)	(181	10)	(189	6)	(191	12)	(192	10)
(193	13)	(195	10)	(203	10)	(205	11)	(206	12)
(207	27)	(211	57)	(212	10)	(219	12)	(220	143)
(221	32)	(222	11)	(225	14)	(227	16)	(262	3)
(277	10)	(298	11)	(299	114)	(300	36)	(301	17)
(314	17)	(315	176)	(316	50)	(317	25)	(359	17)
(360	6)	(367	5)	(403	14)	(404	7)	(462	12)

NAME:13C\_2114.1\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:211003-11-1

RI:2114

RT:13.220

NUM PEAKS: 23

( 70	8)	( 73	1000)	( 74	98)	( 75	120)	( 87	21)
( 98	8)	(103	55)	(116	17)	(131	26)	(132	109)
(133	75)	(146	11)	(147	153)	(173	10)	(175	76)
(176	25)	(220	103)	(221	20)	(285	6)	(299	112)
(315	140)	(316	37)	(415	6)				

NAME:13C\_2125.1\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:213003-11-1

RI:2125

RT:13.290

NUM PEAKS: 42

( 72	22)	( 73	959)	( 74	81)	( 75	61)	( 87	150)
( 89	19)	( 90	21)	(101	69)	(102	21)	(103	35)
(104	78)	(117	12)	(119	54)	(130	26)	(131	30)
(132	38)	(133	40)	(134	14)	(145	15)	(147	176)
(148	30)	(151	13)	(160	16)	(162	25)	(175	1000)
(176	174)	(177	74)	(187	8)	(189	17)	(191	17)
(192	23)	(206	36)	(207	33)	(220	41)	(221	16)
(249	8)	(298	14)	(310	7)	(369	10)	(454	12)
(511	13)	(532	12)						

NAME:13C\_2131.2\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:213001-11-1

RI:2131

RT:13.328

NUM PEAKS: 160

( 72	17)	( 73	1000)	( 74	76)	( 75	67)	( 85	14)
( 86	6)	( 87	16)	( 88	6)	( 89	44)	( 90	24)
( 92	3)	( 95	3)	( 96	3)	( 97	5)	(100	5)
(101	13)	(102	17)	(103	21)	(104	153)	(105	23)
(106	6)	(107	5)	(110	4)	(115	9)	(116	27)
(117	7)	(118	6)	(119	73)	(120	13)	(128	4)
(131	28)	(132	102)	(133	55)	(134	20)	(135	7)
(137	4)	(140	5)	(145	9)	(146	12)	(147	250)

(148	40)	(149	27)	(151	6)	(154	3)	(158	5)
(161	76)	(162	9)	(163	10)	(164	4)	(165	4)
(166	5)	(167	3)	(173	8)	(174	4)	(176	7)
(177	9)	(178	8)	(182	3)	(186	4)	(187	5)
(189	5)	(191	30)	(192	18)	(198	3)	(203	6)
(205	4)	(206	36)	(207	122)	(208	19)	(209	12)
(219	9)	(220	91)	(226	4)	(228	3)	(233	22)
(235	6)	(239	3)	(241	4)	(250	3)	(251	4)
(252	4)	(253	3)	(255	3)	(259	6)	(261	7)
(262	5)	(264	8)	(265	31)	(266	10)	(275	4)
(276	3)	(279	5)	(287	3)	(288	6)	(289	4)
(290	3)	(293	4)	(294	10)	(302	4)	(305	3)
(307	3)	(308	5)	(309	6)	(310	8)	(312	4)
(319	5)	(320	6)	(322	20)	(323	145)	(324	43)
(325	17)	(329	4)	(333	5)	(334	5)	(336	5)
(337	5)	(338	7)	(339	5)	(342	3)	(349	5)
(352	5)	(358	3)	(359	3)	(361	3)	(362	4)
(376	3)	(377	5)	(378	4)	(379	5)	(380	3)
(384	4)	(389	3)	(401	4)	(409	3)	(412	3)
(417	4)	(425	3)	(432	4)	(433	5)	(434	4)
(441	3)	(448	6)	(455	5)	(456	5)	(462	5)
(463	5)	(465	3)	(467	4)	(468	4)	(478	3)
(479	3)	(500	5)	(501	5)	(505	4)	(525	5)
(528	5)	(534	3)	(536	3)	(540	3)	(567	3)

NAME:13C\_2155.1\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:216003-11-1

RI:2155

RT:13.481

NUM PEAKS: 35

( 73	1000)	( 74	95)	( 86	9)	( 87	35)	( 90	22)
( 91	40)	(104	176)	(115	25)	(118	20)	(119	84)
(129	18)	(131	31)	(132	55)	(133	50)	(145	24)
(147	211)	(148	36)	(149	42)	(157	10)	(161	17)
(162	14)	(174	8)	(176	18)	(177	7)	(178	38)
(192	6)	(203	21)	(204	15)	(207	55)	(220	75)
(221	17)	(235	25)	(249	9)	(352	25)	(441	6)

NAME:13C\_2162.2\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:216002-11-1

RI:2162

RT:13.526

NUM PEAKS: 93

( 72	17)	( 73	1000)	( 74	83)	( 75	56)	( 86	6)
( 87	137)	( 88	11)	( 89	26)	( 90	15)	(100	5)
(101	90)	(102	14)	(103	34)	(104	157)	(105	16)
(106	6)	(115	7)	(116	8)	(117	13)	(118	8)
(119	61)	(120	5)	(129	5)	(130	15)	(131	23)
(132	38)	(133	40)	(134	13)	(135	4)	(143	3)
(145	11)	(146	9)	(147	186)	(148	31)	(149	16)
(157	5)	(159	8)	(161	16)	(173	30)	(174	12)
(175	250)	(176	43)	(177	20)	(178	3)	(187	13)
(188	5)	(189	5)	(191	22)	(192	8)	(201	4)
(202	6)	(203	6)	(204	4)	(205	3)	(206	16)
(207	45)	(208	8)	(217	8)	(218	4)	(219	12)
(220	96)	(221	20)	(222	8)	(233	5)	(245	19)
(260	4)	(261	6)	(273	7)	(274	18)	(275	5)
(276	3)	(279	6)	(290	16)	(291	6)	(294	3)

102

(304	5)	(305	4)	(306	4)	(307	3)	(308	8)
(309	4)	(310	17)	(311	5)	(318	10)	(319	12)
(320	5)	(323	6)	(335	6)	(349	11)	(350	3)
(435	3)	(525	5)	(526	4)				

NAME:13C\_2168.8\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:217002-11-1

RI:2169

RT:13.568

NUM PEAKS: 18

( 73	1000)	( 74	83)	( 75	81)	( 87	57)	(101	31)
(103	14)	(132	37)	(133	38)	(145	24)	(147	173)
(148	28)	(149	16)	(174	10)	(191	14)	(192	34)
(220	34)	(262	41)	(442	38)				

NAME:13C\_2179.9\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:218001-11-1

RI:2180

RT:13.638

NUM PEAKS: 57

( 72	24)	( 73	1000)	( 74	88)	( 75	135)	( 87	30)
( 88	12)	( 89	32)	( 90	20)	(100	15)	(103	27)
(104	190)	(105	22)	(115	8)	(116	13)	(117	13)
(118	28)	(119	72)	(130	8)	(131	27)	(132	50)
(133	55)	(134	19)	(145	27)	(146	21)	(147	222)
(148	40)	(149	57)	(150	7)	(161	13)	(162	24)
(163	12)	(176	23)	(177	10)	(178	52)	(179	5)
(188	9)	(189	8)	(203	26)	(205	7)	(207	42)
(220	78)	(221	22)	(222	9)	(234	7)	(235	18)
(236	6)	(249	9)	(275	4)	(319	5)	(320	6)
(322	8)	(348	7)	(351	10)	(352	34)	(353	9)
(528	8)	(533	3)						

NAME:13C\_2217.6\_1313EC11\_9-(Z)-Octadecenoic acid (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:222001-11-1

RI:2218

RT:13.859

NUM PEAKS: 98

( 70	29)	( 71	32)	( 72	257)	( 73	606)	( 74	268)
( 75	1000)	( 76	84)	( 77	49)	( 83	25)	( 84	20)
( 85	102)	( 86	54)	( 87	189)	( 88	122)	( 89	251)
( 90	17)	( 91	14)	( 93	4)	( 96	3)	( 97	4)
( 98	35)	( 99	10)	(100	63)	(101	56)	(102	244)
(103	131)	(104	157)	(105	8)	(106	11)	(113	14)
(114	9)	(115	36)	(116	52)	(117	93)	(118	163)
(119	573)	(120	44)	(121	15)	(128	24)	(130	35)
(131	52)	(132	541)	(133	57)	(134	203)	(135	32)
(136	8)	(143	18)	(144	19)	(145	27)	(146	44)
(148	190)	(149	19)	(150	6)	(158	13)	(159	13)
(160	26)	(161	31)	(162	47)	(163	25)	(164	3)
(173	6)	(174	3)	(176	19)	(177	29)	(178	26)
(179	5)	(180	3)	(188	5)	(190	19)	(191	26)
(192	30)	(193	35)	(194	8)	(205	5)	(206	62)
(208	11)	(221	6)	(222	9)	(223	5)	(236	22)
(237	13)	(238	30)	(250	3)	(251	7)	(252	10)
(253	5)	(266	4)	(268	5)	(281	5)	(282	28)
(283	5)	(284	3)	(355	9)	(356	23)	(357	91)

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(358 12) (359 5) (372 6)

NAME:13C\_2224.7\_1313EC11\_Octadecenoic acid (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:223003-11-1

RI:2225

RT:13.897

NUM PEAKS: 101

( 70 36)	( 71 36)	( 72 267)	( 73 936)	( 74 286)
( 75 1000)	( 76 88)	( 83 30)	( 84 24)	( 85 95)
( 86 57)	( 87 209)	( 88 111)	( 89 245)	( 90 21)
( 96 6)	( 98 39)	( 99 13)	(100 66)	(101 108)
(102 270)	(103 134)	(104 134)	(106 15)	(113 18)
(114 10)	(115 38)	(116 55)	(117 111)	(118 169)
(119 530)	(120 36)	(121 18)	(128 28)	(129 14)
(130 39)	(131 67)	(132 520)	(133 62)	(143 22)
(144 22)	(145 25)	(146 44)	(147 31)	(148 191)
(149 30)	(156 11)	(159 17)	(160 24)	(161 34)
(162 50)	(163 25)	(169 6)	(173 10)	(175 16)
(176 24)	(177 40)	(178 24)	(180 5)	(187 6)
(188 11)	(189 11)	(190 16)	(191 28)	(192 29)
(193 29)	(203 31)	(204 18)	(205 14)	(208 12)
(217 9)	(219 24)	(235 7)	(236 21)	(237 12)
(238 27)	(247 4)	(248 4)	(251 5)	(267 8)
(269 9)	(281 5)	(282 26)	(292 6)	(293 47)
(294 18)	(295 9)	(309 3)	(327 5)	(328 4)
(347 5)	(356 18)	(357 90)	(358 11)	(360 5)
(372 8)	(384 8)	(416 9)	(425 3)	(434 5)
(523 5)				

NAME:13C\_2343.5\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:234001-11-1

RI:2344

RT:14.526

NUM PEAKS: 23

( 72 22)	( 73 1000)	( 74 82)	( 75 101)	(100 25)
(104 58)	(119 22)	(131 26)	(132 34)	(133 50)
(144 18)	(147 145)	(148 29)	(218 21)	(219 14)
(220 370)	(221 64)	(222 29)	(270 25)	(357 18)
(358 45)	(373 10)	(386 6)		

NAME:13C\_2383.1\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:238002-11-1

RI:2383

RT:14.735

NUM PEAKS: 24

( 72 36)	( 73 1000)	( 74 89)	( 75 107)	( 89 24)
( 90 25)	(103 29)	(104 158)	(118 13)	(119 175)
(131 27)	(132 43)	(133 36)	(147 211)	(148 35)
(149 19)	(161 22)	(162 65)	(163 22)	(173 18)
(191 19)	(206 13)	(207 37)	(220 73)	

NAME:13C\_2475.1\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:248002-11-1

RI:2475

RT:15.223

NUM PEAKS: 120

104

( 70	16)	( 72	29)	( 73	1000)	( 74	86)	( 75	131)
( 77	10)	( 82	5)	( 83	7)	( 84	4)	( 86	9)
( 87	12)	( 88	5)	( 89	8)	( 90	14)	( 95	5)
( 96	5)	( 97	5)	( 98	5)	( 99	40)	(100	15)
(101	13)	(102	18)	(103	31)	(104	125)	(105	15)
(106	5)	(112	6)	(113	8)	(114	10)	(115	10)
(116	12)	(117	29)	(118	12)	(119	27)	(120	3)
(125	3)	(126	10)	(127	4)	(128	3)	(129	4)
(130	4)	(131	26)	(132	72)	(133	72)	(135	8)
(139	4)	(140	7)	(141	3)	(144	6)	(145	8)
(146	24)	(147	156)	(148	30)	(149	30)	(153	17)
(154	3)	(155	7)	(156	6)	(158	9)	(159	4)
(160	6)	(161	11)	(164	4)	(168	3)	(169	61)
(170	18)	(171	6)	(173	5)	(174	58)	(175	9)
(176	12)	(177	3)	(178	3)	(183	7)	(184	4)
(185	26)	(186	4)	(191	15)	(192	21)	(193	5)
(196	14)	(199	3)	(206	13)	(213	12)	(214	20)
(215	4)	(218	12)	(219	16)	(220	303)	(221	65)
(222	30)	(223	4)	(227	3)	(228	5)	(229	3)
(233	5)	(234	16)	(235	13)	(236	4)	(241	4)
(242	4)	(243	3)	(245	12)	(248	22)	(249	15)
(250	5)	(255	3)	(257	5)	(263	6)	(264	62)
(265	11)	(266	5)	(270	11)	(271	7)	(272	3)
(301	12)	(302	3)	(317	7)	(353	3)	(450	3)

NAME:13C\_2732.8\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:273002-11-1

RI:2733

RT:16.587

NUM PEAKS: 64

( 71	6)	( 72	16)	( 73	1000)	( 74	89)	( 75	85)
( 84	5)	( 86	25)	( 87	11)	( 89	31)	( 90	16)
(101	11)	(102	8)	(103	27)	(104	123)	(105	36)
(106	8)	(115	10)	(116	9)	(117	9)	(118	13)
(119	76)	(121	5)	(131	21)	(132	90)	(133	56)
(134	21)	(145	6)	(146	23)	(147	259)	(148	46)
(149	27)	(160	15)	(161	16)	(162	83)	(163	20)
(173	8)	(174	52)	(175	8)	(178	8)	(189	5)
(190	10)	(191	25)	(192	34)	(193	9)	(205	9)
(206	244)	(207	107)	(208	26)	(220	122)	(221	32)
(222	11)	(234	7)	(248	44)	(249	12)	(275	3)
(277	23)	(278	9)	(294	6)	(323	18)	(366	22)
(367	132)	(368	40)	(369	18)	(396	4)		

NAME:13C\_2814.8\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:281001-11-1

RI:2815

RT:17.009

NUM PEAKS: 53

( 72	14)	( 73	1000)	( 74	83)	( 75	81)	( 87	9)
( 89	25)	(103	40)	(104	74)	(105	20)	(106	6)
(115	10)	(118	18)	(119	52)	(131	22)	(132	81)
(133	56)	(134	20)	(135	7)	(145	10)	(146	18)
(147	273)	(148	47)	(149	30)	(161	17)	(162	67)
(164	30)	(174	37)	(176	6)	(191	32)	(192	42)
(206	264)	(207	106)	(208	28)	(219	9)	(220	80)
(221	176)	(222	45)	(223	20)	(236	6)	(248	19)
(249	11)	(264	7)	(279	6)	(281	30)	(282	9)

105

(295 48) (296 16) (323 9) (324 5) (355 8)  
(367 85) (368 29) (369 34)

NAME:13C\_2825.9\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:283001-11-1

RI:2826

RT:17.058

NUM PEAKS: 36

( 70 27) ( 72 174) ( 73 189) ( 74 1000) ( 83 45)  
( 86 53) ( 87 511) ( 88 20) ( 89 18) ( 98 59)  
(100 109) (101 43) (102 144) (104 8) (113 35)  
(114 12) (115 71) (117 59) (128 31) (129 16)  
(130 92) (131 19) (132 58) (143 20) (144 20)  
(145 49) (146 75) (147 59) (158 26) (160 44)  
(171 7) (173 15) (175 8) (203 11) (205 10)  
(218 10)

NAME:13C\_2872.6\_1313EC11\_Isomaltose methoxyamine (8TMS); alpha-D-Glc-(1,6)-D-Glc (8TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:287001-11-1

RI:2873

RT:17.266

NUM PEAKS: 58

( 73 1000) ( 74 87) ( 75 98) ( 76 9) ( 86 17)  
( 87 12) ( 88 5) ( 89 30) ( 90 12) (101 21)  
(102 13) (103 42) (104 112) (105 28) (115 14)  
(116 13) (118 21) (119 67) (130 7) (131 21)  
(132 115) (133 65) (134 23) (135 9) (145 11)  
(146 21) (147 236) (148 41) (149 27) (160 19)  
(161 26) (162 89) (163 17) (164 25) (173 8)  
(174 61) (175 10) (177 9) (190 6) (191 35)  
(192 49) (205 13) (206 207) (207 59) (208 22)  
(220 115) (234 13) (235 17) (248 29) (249 14)  
(277 23) (278 9) (279 8) (323 16) (366 24)  
(367 140) (368 46) (369 21)

NAME:13C\_2907.8\_1313EC11\_Isomaltose methoxyamine {BP} (8TMS); alpha-D-Glc-(1,6)-D-Glc (8TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:291002-11-1

RI:2908

RT:17.423

NUM PEAKS: 72

( 72 14) ( 73 1000) ( 74 83) ( 75 111) ( 79 18)  
( 86 23) ( 87 14) ( 89 24) ( 90 13) ( 94 12)  
( 98 13) (102 23) (103 44) (104 140) (105 26)  
(115 18) (117 12) (118 12) (119 48) (126 10)  
(131 21) (132 93) (133 55) (134 37) (146 26)  
(147 221) (148 40) (160 13) (161 23) (162 74)  
(164 33) (165 15) (174 61) (178 9) (191 26)  
(192 41) (204 12) (206 200) (207 63) (212 9)  
(220 87) (221 19) (233 9) (235 34) (248 31)  
(251 10) (259 8) (262 10) (270 8) (279 14)  
(289 11) (308 20) (309 12) (310 15) (314 9)  
(322 10) (340 12) (366 21) (367 128) (368 43)  
(381 18) (389 14) (397 8) (411 12) (412 7)  
(420 9) (437 17) (448 15) (534 9) (536 10)  
(545 9) (577 6)

106

NAME:13C\_2932.1\_1313EC11

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:293001-11-1

RI:2932

RT:17.530

NUM PEAKS: 96

( 72	14)	( 73	1000)	( 74	83)	( 75	83)	( 76	4)
( 81	8)	( 86	10)	( 87	8)	( 88	4)	( 89	5)
( 90	6)	(101	7)	(102	7)	(103	79)	(104	81)
(105	10)	(111	3)	(115	8)	(116	6)	(117	9)
(118	15)	(119	36)	(129	62)	(130	8)	(131	22)
(132	78)	(133	64)	(134	10)	(135	5)	(143	11)
(144	4)	(145	7)	(146	15)	(147	299)	(148	47)
(149	32)	(150	3)	(157	7)	(160	8)	(161	14)
(174	28)	(175	7)	(176	4)	(177	6)	(178	3)
(189	9)	(190	6)	(191	166)	(192	66)	(193	19)
(194	3)	(204	15)	(205	22)	(206	591)	(207	108)
(208	46)	(209	5)	(217	49)	(218	11)	(219	9)
(220	90)	(221	38)	(222	12)	(230	16)	(231	6)
(232	3)	(233	3)	(234	4)	(235	7)	(243	6)
(247	4)	(248	15)	(249	5)	(265	4)	(271	3)
(277	7)	(278	3)	(291	5)	(293	7)	(294	5)
(304	4)	(305	16)	(306	6)	(307	3)	(308	8)
(309	3)	(318	9)	(319	6)	(322	4)	(323	4)
(336	3)	(343	5)	(367	20)	(368	6)	(433	10)
(434	5)								

NAME:13C\_2517.7\_1313EC11

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:252002-11-1

RI:2518

RT:15.448

NUM PEAKS: 254

( 70	14)	( 71	36)	( 72	107)	( 73	1000)	( 74	97)
( 75	126)	( 76	10)	( 77	7)	( 78	3)	( 79	3)
( 83	10)	( 84	7)	( 85	32)	( 86	12)	( 87	15)
( 88	11)	( 89	32)	( 90	19)	( 91	6)	( 93	4)
( 96	3)	( 97	6)	( 98	7)	( 99	9)	(100	11)
(101	53)	(102	26)	(103	33)	(104	185)	(105	20)
(106	6)	(108	3)	(111	6)	(112	4)	(113	13)
(114	9)	(115	10)	(116	11)	(117	9)	(118	11)
(119	57)	(120	6)	(121	3)	(124	3)	(125	3)
(127	4)	(129	14)	(130	9)	(131	27)	(132	45)
(133	51)	(134	18)	(135	9)	(137	3)	(138	3)
(140	4)	(141	7)	(142	7)	(143	6)	(144	9)
(145	22)	(146	20)	(147	191)	(148	32)	(149	20)
(150	4)	(151	4)	(153	3)	(154	3)	(155	4)
(157	4)	(158	8)	(159	9)	(160	90)	(161	21)
(162	12)	(163	8)	(164	3)	(169	3)	(171	5)
(172	9)	(173	11)	(174	8)	(175	25)	(176	38)
(177	16)	(178	5)	(180	4)	(183	3)	(186	6)
(187	7)	(188	7)	(189	6)	(190	6)	(191	72)
(192	17)	(193	7)	(195	3)	(196	5)	(197	3)
(198	3)	(201	4)	(202	4)	(203	7)	(204	8)
(205	5)	(206	15)	(207	28)	(208	7)	(209	5)
(212	4)	(213	5)	(214	4)	(215	3)	(216	6)
(217	3)	(218	6)	(219	14)	(220	114)	(221	20)
(222	9)	(223	3)	(226	3)	(227	4)	(230	3)
(231	7)	(232	16)	(233	8)	(234	6)	(235	6)



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(236	4)	(239	3)	(244	3)	(245	7)	(246	4)
(247	4)	(248	9)	(249	6)	(250	4)	(253	5)
(257	3)	(260	3)	(261	4)	(262	5)	(263	3)
(264	5)	(265	3)	(266	3)	(267	3)	(268	3)
(274	3)	(276	4)	(277	7)	(278	4)	(279	12)
(280	4)	(289	3)	(293	4)	(294	6)	(295	3)
(296	3)	(301	4)	(302	3)	(304	3)	(305	4)
(306	7)	(307	4)	(308	4)	(309	3)	(310	5)
(313	3)	(319	3)	(320	8)	(321	3)	(322	5)
(323	5)	(324	5)	(325	3)	(326	3)	(333	3)
(334	4)	(335	6)	(336	5)	(337	3)	(338	3)
(339	3)	(341	3)	(344	3)	(347	3)	(349	5)
(350	7)	(351	21)	(352	9)	(353	3)	(361	3)
(363	3)	(364	5)	(365	4)	(367	3)	(368	3)
(372	3)	(376	3)	(377	3)	(380	4)	(381	12)
(382	11)	(383	3)	(387	4)	(388	3)	(394	3)
(395	4)	(396	4)	(397	3)	(409	3)	(412	3)
(422	6)	(423	16)	(424	10)	(425	5)	(427	3)
(437	3)	(439	3)	(442	3)	(447	3)	(449	3)
(450	3)	(452	6)	(453	20)	(454	56)	(455	26)
(456	10)	(457	3)	(460	3)	(467	3)	(470	3)
(480	3)	(481	3)	(491	3)	(492	3)	(503	3)
(506	3)	(508	3)	(513	4)	(514	4)	(515	3)
(516	4)	(519	3)	(522	3)	(526	4)	(535	3)
(536	3)	(542	3)	(544	3)	(569	3)		

NAME:13C\_2491.6\_1313EC11

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:249001-11-1

RI:2492

RT:15.310

NUM PEAKS: 205

( 70	15)	( 71	16)	( 72	60)	( 73	1000)	( 74	66)
( 75	104)	( 77	10)	( 82	4)	( 85	15)	( 86	7)
( 87	5)	( 88	3)	( 89	14)	( 90	10)	( 92	5)
( 93	3)	( 96	7)	( 98	3)	( 99	10)	(100	11)
(101	27)	(102	12)	(103	28)	(104	121)	(105	16)
(106	7)	(108	5)	(110	3)	(111	4)	(113	3)
(114	7)	(115	4)	(116	6)	(117	7)	(118	5)
(119	27)	(123	4)	(126	6)	(128	3)	(129	7)
(131	27)	(132	16)	(133	42)	(134	7)	(139	6)
(141	4)	(142	6)	(143	6)	(144	4)	(145	22)
(146	13)	(147	208)	(148	41)	(149	22)	(150	3)
(151	3)	(155	4)	(158	4)	(159	3)	(160	52)
(161	16)	(162	7)	(163	6)	(168	4)	(169	10)
(170	4)	(171	4)	(172	5)	(173	5)	(174	16)
(175	11)	(176	25)	(177	5)	(185	8)	(186	3)
(188	7)	(189	4)	(191	32)	(192	12)	(193	5)
(194	4)	(195	3)	(196	3)	(202	4)	(203	6)
(204	3)	(205	8)	(206	4)	(207	33)	(208	8)
(210	4)	(211	3)	(213	3)	(214	6)	(216	5)
(218	3)	(219	6)	(220	98)	(221	52)	(222	14)
(223	7)	(231	4)	(232	11)	(233	5)	(234	7)
(235	5)	(236	3)	(237	3)	(239	3)	(245	3)
(248	4)	(249	5)	(252	6)	(256	4)	(257	4)
(258	4)	(261	5)	(263	3)	(264	12)	(265	5)
(266	4)	(267	7)	(270	4)	(273	4)	(274	3)
(275	4)	(276	7)	(277	3)	(279	10)	(280	3)
(281	20)	(282	3)	(283	3)	(288	5)	(295	6)
(309	3)	(310	4)	(317	5)	(319	8)	(320	9)

108

(321	3)	(323	5)	(325	8)	(326	3)	(329	3)
(334	3)	(335	3)	(341	7)	(342	4)	(347	3)
(348	4)	(350	5)	(351	19)	(352	7)	(353	3)
(355	18)	(356	9)	(357	4)	(364	3)	(374	4)
(378	4)	(381	12)	(382	6)	(383	3)	(389	3)
(390	3)	(394	4)	(398	3)	(400	3)	(401	4)
(418	3)	(419	3)	(422	5)	(423	12)	(424	6)
(425	4)	(429	5)	(430	6)	(431	5)	(434	3)
(435	5)	(438	3)	(439	4)	(449	5)	(450	4)
(452	7)	(453	19)	(454	53)	(455	20)	(456	8)
(459	4)	(471	4)	(474	5)	(481	6)	(490	4)
(491	5)	(505	4)	(528	3)	(534	3)	(541	3)
(543	3)	(557	3)	(562	4)	(569	3)	(592	3)

NAME:13C\_3307.7\_1313EC07\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:331001-11-1

RI:3308

RT:19.156

NUM PEAKS: 141

( 72	135)	( 73	765)	( 74	279)	( 75	626)	( 76	387)
( 77	49)	( 82	9)	( 83	13)	( 85	29)	( 86	28)
( 87	205)	( 88	75)	( 89	209)	( 90	49)	( 91	189)
( 93	17)	( 98	19)	(100	45)	(101	29)	(102	198)
(103	128)	(104	381)	(105	53)	(106	38)	(113	12)
(115	38)	(116	38)	(117	55)	(118	102)	(119	144)
(120	23)	(121	16)	(122	7)	(128	15)	(129	12)
(130	21)	(131	34)	(132	1000)	(133	149)	(134	283)
(135	40)	(136	24)	(141	12)	(142	9)	(145	24)
(147	90)	(148	847)	(149	109)	(150	39)	(156	9)
(157	7)	(158	9)	(160	11)	(161	23)	(162	17)
(163	26)	(164	47)	(165	298)	(171	11)	(175	15)
(177	19)	(178	15)	(179	26)	(183	6)	(189	7)
(192	19)	(193	37)	(194	80)	(195	10)	(207	82)
(208	13)	(209	9)	(211	6)	(220	7)	(221	8)
(222	18)	(224	9)	(229	8)	(230	10)	(232	8)
(234	8)	(237	33)	(238	43)	(239	460)	(240	36)
(241	19)	(242	23)	(244	9)	(248	10)	(250	8)
(252	25)	(253	30)	(254	30)	(255	118)	(256	8)
(267	35)	(282	10)	(285	14)	(289	11)	(291	8)
(299	8)	(308	10)	(309	7)	(311	9)	(312	15)
(313	26)	(314	57)	(315	9)	(325	7)	(328	25)
(329	113)	(330	17)	(331	8)	(332	13)	(334	8)
(343	10)	(344	24)	(345	27)	(357	11)	(358	11)
(375	7)	(381	9)	(391	9)	(392	9)	(402	9)
(403	35)	(404	33)	(408	6)	(428	11)	(461	12)
(493	5)	(497	7)	(498	7)	(501	6)	(508	7)
(511	8)	(523	6)	(569	11)	(570	24)	(571	11)
(573	4)								

NAME:13C\_3401.6\_1313EC07\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:340002-11-1

RI:3402

RT:19.533

NUM PEAKS: 214

( 70	188)	( 71	791)	( 72	275)	( 73	872)	( 74	1000)
( 75	556)	( 76	73)	( 77	48)	( 80	27)	( 81	45)
( 82	68)	( 83	290)	( 84	120)	( 85	663)	( 86	70)
( 87	255)	( 88	54)	( 89	120)	( 91	28)	( 95	20)

109

( 96 56)	( 97 193)	( 98 289)	( 99 243)	(100 230)
(101 48)	(102 278)	(103 49)	(104 32)	(106 7)
(109 9)	(110 34)	(111 108)	(112 70)	(113 399)
(114 43)	(115 196)	(116 27)	(117 179)	(118 11)
(119 48)	(120 16)	(123 13)	(124 73)	(125 75)
(126 120)	(127 124)	(128 191)	(129 35)	(130 133)
(131 55)	(132 358)	(133 43)	(134 36)	(137 35)
(138 70)	(139 100)	(140 67)	(141 228)	(142 55)
(143 167)	(144 87)	(145 429)	(146 76)	(148 18)
(149 12)	(152 54)	(153 46)	(154 103)	(155 92)
(156 151)	(157 85)	(158 143)	(159 43)	(160 100)
(162 31)	(164 23)	(165 17)	(166 21)	(167 42)
(168 48)	(169 114)	(170 36)	(171 129)	(172 38)
(173 114)	(174 29)	(175 57)	(176 9)	(177 23)
(178 15)	(179 13)	(180 16)	(181 17)	(182 30)
(183 38)	(184 57)	(185 34)	(186 99)	(187 38)
(188 94)	(189 21)	(190 37)	(191 9)	(192 14)
(196 20)	(197 53)	(198 12)	(199 58)	(200 49)
(201 107)	(202 30)	(203 47)	(207 17)	(208 10)
(210 10)	(211 28)	(212 24)	(213 16)	(214 42)
(215 12)	(216 56)	(217 19)	(218 41)	(219 26)
(220 46)	(221 11)	(224 12)	(225 19)	(226 12)
(227 15)	(228 11)	(229 33)	(230 16)	(231 26)
(232 11)	(234 13)	(235 34)	(238 9)	(239 17)
(240 13)	(241 8)	(243 8)	(245 10)	(246 20)
(251 12)	(253 14)	(256 14)	(259 63)	(260 10)
(261 46)	(262 18)	(263 19)	(266 14)	(272 8)
(273 10)	(274 24)	(275 18)	(276 29)	(277 51)
(278 22)	(282 10)	(286 10)	(288 11)	(289 11)
(290 9)	(291 12)	(292 16)	(302 14)	(309 10)
(319 14)	(320 9)	(322 10)	(323 8)	(324 8)
(327 10)	(332 11)	(334 10)	(335 13)	(338 14)
(342 12)	(349 16)	(361 7)	(377 11)	(379 12)
(380 15)	(391 9)	(392 12)	(394 10)	(405 11)
(406 13)	(407 43)	(422 13)	(423 25)	(424 12)
(429 15)	(442 6)	(451 11)	(452 9)	(455 7)
(468 13)	(476 11)	(495 7)	(499 9)	(512 24)
(513 45)	(514 13)	(518 8)	(523 6)	(545 10)
(546 9)	(547 8)	(566 8)	(592 6)	

NAME:13C\_3494.1\_1313EC07\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:349001-11-1

RI:3494

RT:19.905

NUM PEAKS: 70

( 70 20)	( 72 144)	( 73 864)	( 74 282)	( 75 770)
( 76 360)	( 77 71)	( 86 28)	( 87 149)	( 88 94)
( 89 300)	( 90 62)	( 91 155)	( 92 14)	( 93 25)
(100 23)	(101 40)	(102 230)	(103 134)	(104 457)
(105 36)	(106 47)	(116 37)	(117 129)	(118 107)
(119 148)	(120 30)	(122 20)	(130 19)	(131 25)
(132 1000)	(133 166)	(134 281)	(135 29)	(136 22)
(146 21)	(147 65)	(148 858)	(149 130)	(150 20)
(162 23)	(168 12)	(177 35)	(179 15)	(192 26)
(193 51)	(194 114)	(195 217)	(207 78)	(222 17)
(252 15)	(255 43)	(267 38)	(268 49)	(269 376)
(270 30)	(271 16)	(284 13)	(285 45)	(328 26)
(329 140)	(343 21)	(344 73)	(345 40)	(403 32)
(404 43)	(424 12)	(425 12)	(473 10)	(572 9)

NAME:13C\_3334.7\_1313EC07

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:334001-11-1

RI:3335

RT:19.264

NUM PEAKS: 191

( 70 67)	( 71 41)	( 72 226)	( 73 1000)	( 74 566)
( 75 796)	( 76 188)	( 77 53)	( 80 29)	( 82 43)
( 83 123)	( 84 46)	( 85 184)	( 86 56)	( 87 294)
( 88 66)	( 89 119)	( 91 57)	( 92 23)	( 93 24)
( 94 21)	( 95 33)	( 96 37)	( 97 46)	( 98 274)
( 99 40)	(100 189)	(101 54)	(102 240)	(103 57)
(104 89)	(105 16)	(111 39)	(113 267)	(114 31)
(115 147)	(116 53)	(117 137)	(118 34)	(119 51)
(123 25)	(124 120)	(125 33)	(126 138)	(127 75)
(128 328)	(129 63)	(130 137)	(131 43)	(132 156)
(133 59)	(134 156)	(135 21)	(136 20)	(137 82)
(138 184)	(139 182)	(140 57)	(141 209)	(142 70)
(143 142)	(144 47)	(145 84)	(146 45)	(148 118)
(150 22)	(151 40)	(152 155)	(153 144)	(154 364)
(155 109)	(156 333)	(157 62)	(158 100)	(159 24)
(160 57)	(161 21)	(162 20)	(164 56)	(166 63)
(167 148)	(168 80)	(169 268)	(170 141)	(171 212)
(172 49)	(173 77)	(174 33)	(175 60)	(176 16)
(177 19)	(178 51)	(179 28)	(180 46)	(181 49)
(182 126)	(183 58)	(184 158)	(185 58)	(186 88)
(187 31)	(188 32)	(189 29)	(190 16)	(192 24)
(193 38)	(194 19)	(195 55)	(196 37)	(197 106)
(198 48)	(199 126)	(201 45)	(203 29)	(204 23)
(210 50)	(211 46)	(212 105)	(213 60)	(214 108)
(215 23)	(217 17)	(219 42)	(220 19)	(222 27)
(225 23)	(226 31)	(227 128)	(228 43)	(229 54)
(230 29)	(232 15)	(240 23)	(241 24)	(242 53)
(243 50)	(244 65)	(246 24)	(251 17)	(252 15)
(253 12)	(256 15)	(257 16)	(258 15)	(259 35)
(260 18)	(261 30)	(271 24)	(272 58)	(273 15)
(284 17)	(285 26)	(287 19)	(289 11)	(292 13)
(300 17)	(302 18)	(309 22)	(334 15)	(342 9)
(350 16)	(352 14)	(362 38)	(363 83)	(364 112)
(365 15)	(368 14)	(377 20)	(379 16)	(380 14)
(386 20)	(390 28)	(391 108)	(392 163)	(393 42)
(395 13)	(405 22)	(406 16)	(407 33)	(408 33)
(435 14)	(444 17)	(483 21)	(484 15)	(494 14)
(497 32)	(498 35)	(499 13)	(509 17)	(533 13)
(568 8)				

NAME:13C\_3347.5\_1313EC07

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:335001-11-1

RI:3348

RT:19.315

NUM PEAKS: 140

( 70 55)	( 71 36)	( 72 231)	( 73 535)	( 74 433)
( 75 1000)	( 76 66)	( 77 32)	( 82 27)	( 83 125)
( 84 52)	( 85 242)	( 86 45)	( 87 264)	( 88 32)
( 89 123)	( 90 83)	( 96 18)	( 97 27)	( 98 317)
( 99 50)	(100 206)	(101 59)	(102 190)	(103 26)
(104 35)	(111 31)	(112 34)	(113 297)	(114 55)
(115 243)	(116 33)	(117 83)	(123 12)	(124 73)

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(125	24)	(126	123)	(127	39)	(128	179)	(129	44)
(130	85)	(131	30)	(132	64)	(133	12)	(136	10)
(137	29)	(138	73)	(139	100)	(140	37)	(141	180)
(142	51)	(143	131)	(144	45)	(145	64)	(146	17)
(152	53)	(153	47)	(154	108)	(155	50)	(156	173)
(157	58)	(158	117)	(159	19)	(160	54)	(161	55)
(162	18)	(166	21)	(167	39)	(168	21)	(169	88)
(170	42)	(171	145)	(172	29)	(173	70)	(174	24)
(175	25)	(178	8)	(180	11)	(181	18)	(182	35)
(184	66)	(185	18)	(186	70)	(187	23)	(188	24)
(189	17)	(190	26)	(191	8)	(195	8)	(197	26)
(198	15)	(199	63)	(200	27)	(201	39)	(202	13)
(203	31)	(204	24)	(212	34)	(213	19)	(214	43)
(216	36)	(217	27)	(218	15)	(226	13)	(227	51)
(228	27)	(229	112)	(230	14)	(231	15)	(242	21)
(243	28)	(244	78)	(245	27)	(257	16)	(258	14)
(259	11)	(261	12)	(270	6)	(271	21)	(272	86)
(276	7)	(278	7)	(302	25)	(303	9)	(317	16)
(347	20)	(348	11)	(361	46)	(362	210)	(363	44)
(364	14)	(391	15)	(392	29)	(393	18)	(407	20)
(408	51)	(409	13)	(482	17)	(483	9)	(530	8)

NAME:13C\_3353.6\_1313EC07\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:335002-11-1

RI:3354

RT:19.340

NUM PEAKS: 166

( 70	62)	( 71	62)	( 72	175)	( 73	888)	( 74	215)
( 75	1000)	( 76	232)	( 77	67)	( 83	148)	( 84	65)
( 85	190)	( 86	23)	( 87	321)	( 88	34)	( 89	79)
( 90	28)	( 91	37)	( 93	37)	( 97	41)	( 98	344)
( 99	52)	(100	177)	(101	42)	(102	209)	(104	129)
(105	34)	(106	29)	(110	30)	(111	47)	(112	31)
(113	284)	(114	43)	(115	169)	(117	104)	(118	51)
(119	23)	(121	17)	(124	53)	(125	26)	(126	88)
(127	44)	(128	159)	(129	72)	(130	92)	(132	103)
(134	48)	(137	43)	(138	67)	(139	82)	(140	48)
(141	161)	(142	41)	(143	126)	(144	100)	(145	109)
(146	36)	(147	181)	(150	32)	(152	76)	(153	64)
(154	120)	(155	63)	(156	141)	(157	49)	(158	145)
(160	60)	(161	17)	(162	25)	(163	24)	(165	30)
(166	46)	(169	102)	(170	57)	(171	120)	(172	25)
(173	79)	(174	23)	(179	28)	(184	37)	(185	26)
(186	84)	(188	57)	(190	19)	(192	34)	(197	24)
(198	25)	(199	44)	(200	51)	(206	50)	(207	74)
(212	40)	(213	28)	(214	51)	(215	56)	(216	27)
(217	16)	(218	27)	(220	61)	(221	117)	(222	31)
(223	42)	(227	33)	(228	58)	(229	198)	(230	26)
(231	33)	(233	20)	(245	41)	(246	104)	(253	37)
(259	22)	(274	226)	(276	31)	(280	18)	(281	49)
(293	30)	(300	25)	(308	19)	(316	26)	(320	39)
(333	23)	(342	18)	(357	30)	(375	22)	(377	28)
(379	24)	(381	32)	(382	19)	(394	46)	(400	26)
(417	33)	(420	34)	(421	20)	(425	16)	(426	31)
(429	25)	(430	23)	(433	13)	(440	25)	(441	37)
(445	27)	(449	16)	(450	23)	(455	30)	(457	24)
(484	38)	(487	22)	(499	51)	(500	109)	(501	42)
(502	17)	(515	29)	(516	39)	(520	16)	(524	29)
(525	21)	(529	18)	(534	18)	(537	18)	(545	17)

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(568 12) (569 10) (574 11) (587 11) (590 14)  
 (599 7)

NAME:13C\_2654.6\_1313EC07\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:266001-11-1

RI:2655

RT:16.184

NUM PEAKS: 100

( 70 7) ( 71 12) ( 72 70) ( 73 1000) ( 74 328)  
 ( 75 86) ( 85 29) ( 86 16) ( 87 60) ( 88 13)  
 ( 89 33) ( 90 12) ( 99 8) (100 14) (101 27)  
 (102 32) (103 86) (104 312) (105 15) (106 8)  
 (114 8) (115 28) (116 13) (118 24) (119 67)  
 (120 6) (128 10) (129 7) (130 10) (131 69)  
 (132 55) (133 204) (134 8) (143 8) (144 14)  
 (145 13) (146 14) (147 210) (148 31) (149 15)  
 (157 11) (158 7) (159 20) (160 17) (172 11)  
 (173 33) (174 27) (175 30) (176 49) (177 15)  
 (187 18) (189 13) (190 28) (191 19) (192 9)  
 (202 5) (203 16) (204 23) (205 10) (206 32)  
 (207 24) (208 4) (213 11) (216 6) (218 9)  
 (219 9) (220 37) (221 8) (224 4) (231 9)  
 (232 12) (233 10) (245 5) (246 9) (247 12)  
 (273 6) (274 41) (275 22) (276 37) (277 15)  
 (294 4) (295 7) (301 4) (302 12) (303 60)  
 (304 15) (306 12) (307 61) (308 7) (320 10)  
 (334 22) (335 18) (336 42) (337 12) (338 7)  
 (393 15) (410 4) (482 6) (483 17) (484 7)

NAME:13C\_2689.6\_1313EC07\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:269002-11-1

RI:2690

RT:16.369

NUM PEAKS: 259

( 70 5) ( 71 13) ( 72 10) ( 73 1000) ( 74 86)  
 ( 75 48) ( 76 13) ( 77 3) ( 78 3) ( 82 4)  
 ( 83 3) ( 84 21) ( 85 20) ( 86 47) ( 87 12)  
 ( 88 13) ( 90 19) ( 93 18) ( 96 7) ( 97 28)  
 ( 99 20) (100 13) (101 7) (103 42) (104 287)  
 (105 56) (108 19) (115 12) (116 4) (117 37)  
 (118 18) (119 23) (120 7) (121 4) (127 17)  
 (128 4) (130 6) (132 216) (133 51) (134 6)  
 (139 7) (140 4) (143 19) (145 9) (146 26)  
 (147 259) (148 70) (149 12) (150 20) (151 4)  
 (154 7) (156 22) (157 11) (160 66) (161 43)  
 (164 8) (168 8) (169 3) (170 9) (171 14)  
 (174 187) (175 32) (176 29) (177 34) (178 5)  
 (179 8) (182 4) (184 11) (187 9) (188 7)  
 (189 6) (190 8) (191 81) (192 427) (193 69)  
 (194 17) (199 16) (200 26) (201 11) (204 7)  
 (205 38) (206 335) (209 4) (215 8) (216 16)  
 (217 12) (220 231) (221 32) (222 10) (231 11)  
 (232 9) (233 7) (235 36) (236 13) (238 4)  
 (244 19) (246 4) (247 15) (248 66) (249 7)  
 (250 5) (251 8) (252 9) (254 6) (255 13)  
 (256 7) (257 19) (258 8) (259 4) (260 3)  
 (262 12) (263 6) (264 22) (265 7) (266 3)  
 (272 5) (274 5) (278 6) (282 21) (285 4)



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NAME:13C\_3185.4\_1313EC07

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:318001-11-1

RI:3185

RT:18.659

NUM PEAKS: 138

( 70	5)	( 71	5)	( 72	17)	( 73	1000)	( 74	94)
( 75	99)	( 76	6)	( 77	6)	( 84	3)	( 85	8)
( 86	36)	( 87	13)	( 88	4)	( 89	9)	( 90	6)
( 98	4)	(100	3)	(101	6)	(102	9)	(103	22)
(104	86)	(105	9)	(106	3)	(114	5)	(115	35)
(116	17)	(117	8)	(118	13)	(119	32)	(130	6)
(131	21)	(132	133)	(133	73)	(134	17)	(135	12)
(137	4)	(144	6)	(145	8)	(146	22)	(147	233)
(148	39)	(149	28)	(151	5)	(158	8)	(159	5)
(160	37)	(161	19)	(162	3)	(173	5)	(174	48)
(175	10)	(176	9)	(177	7)	(178	7)	(181	6)
(186	3)	(187	3)	(188	8)	(189	16)	(190	4)
(191	31)	(192	36)	(193	13)	(195	6)	(203	3)
(204	4)	(205	10)	(206	54)	(207	27)	(208	7)
(209	4)	(210	3)	(211	52)	(212	11)	(213	4)
(218	5)	(219	3)	(220	98)	(221	30)	(222	11)
(225	8)	(227	19)	(232	3)	(233	5)	(234	6)
(235	9)	(236	4)	(243	11)	(245	3)	(246	4)
(247	23)	(248	32)	(249	12)	(250	5)	(255	5)
(261	4)	(262	5)	(275	3)	(276	30)	(277	187)
(278	34)	(279	16)	(283	4)	(285	7)	(294	7)
(298	7)	(299	89)	(300	24)	(301	13)	(308	6)
(309	3)	(313	4)	(314	13)	(315	194)	(316	52)
(317	26)	(318	4)	(322	3)	(323	4)	(338	7)
(359	5)	(366	3)	(367	22)	(368	6)	(373	7)
(386	13)	(387	70)	(388	25)	(389	15)	(390	3)
(428	4)	(429	16)	(430	5)	(431	3)	(518	7)
(519	21)	(520	9)	(521	6)				

NAME:13C\_2718.2\_1313EC07

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:272002-11-1

RI:2718

RT:16.522

NUM PEAKS: 159

( 70	5)	( 71	7)	( 72	16)	( 73	1000)	( 74	91)
( 75	76)	( 76	3)	( 77	15)	( 79	3)	( 84	3)
( 85	8)	( 86	13)	( 87	7)	( 88	4)	( 89	26)
( 90	6)	( 91	6)	( 98	3)	( 99	3)	(100	3)
(101	7)	(102	12)	(103	41)	(104	9)	(105	11)
(106	3)	(107	4)	(114	3)	(115	14)	(116	12)
(117	8)	(118	15)	(119	12)	(121	6)	(129	4)
(130	5)	(131	18)	(132	79)	(133	73)	(134	15)
(135	21)	(136	3)	(137	11)	(144	6)	(145	26)
(146	9)	(147	119)	(148	19)	(149	15)	(150	3)
(151	9)	(158	4)	(159	4)	(160	5)	(161	7)
(163	5)	(165	4)	(167	3)	(173	5)	(174	5)
(175	4)	(176	28)	(177	6)	(179	3)	(181	13)
(182	3)	(183	5)	(186	8)	(187	4)	(188	3)
(189	4)	(190	3)	(191	14)	(192	16)	(193	16)
(194	4)	(195	14)	(196	3)	(197	4)	(202	6)
(203	4)	(204	3)	(205	4)	(206	24)	(207	23)
(208	6)	(209	6)	(210	3)	(211	74)	(212	12)
(213	7)	(218	4)	(219	5)	(220	88)	(221	18)



115

(222	8)	(225	30)	(226	7)	(227	19)	(228	3)
(233	4)	(234	5)	(237	9)	(238	3)	(241	3)
(242	4)	(243	4)	(248	3)	(255	5)	(268	3)
(269	3)	(274	5)	(275	3)	(276	4)	(283	7)
(284	4)	(285	8)	(298	17)	(299	157)	(300	47)
(301	24)	(302	5)	(306	3)	(313	4)	(314	19)
(315	153)	(316	44)	(317	23)	(318	4)	(329	4)
(343	6)	(355	3)	(356	14)	(357	7)	(358	8)
(359	25)	(360	8)	(361	4)	(371	3)	(372	5)
(373	6)	(374	3)	(385	4)	(386	28)	(387	100)
(388	41)	(389	22)	(390	5)	(416	6)	(417	16)
(418	6)	(419	3)	(450	3)	(451	6)	(452	3)
(461	4)	(462	12)	(463	6)	(464	3)		

NAME:13C\_2724.4\_1313EC07

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:272001-11-1

RI:2724

RT:16.554

NUM PEAKS: 143

( 70	6)	( 71	6)	( 72	17)	( 73	1000)	( 74	92)
( 75	75)	( 76	4)	( 77	15)	( 85	9)	( 86	11)
( 87	6)	( 88	3)	( 89	36)	( 90	7)	( 91	7)
( 98	3)	( 99	3)	(100	3)	(101	8)	(102	12)
(103	44)	(104	15)	(105	13)	(106	3)	(107	5)
(114	3)	(115	14)	(116	10)	(117	9)	(118	14)
(119	13)	(120	3)	(121	6)	(123	3)	(129	4)
(130	5)	(131	18)	(132	94)	(133	74)	(134	17)
(135	22)	(136	3)	(137	12)	(144	5)	(145	30)
(146	9)	(147	109)	(148	17)	(149	14)	(151	10)
(158	3)	(159	4)	(160	4)	(161	8)	(163	6)
(165	4)	(167	3)	(173	4)	(175	4)	(176	34)
(177	7)	(179	3)	(181	14)	(182	3)	(183	4)
(186	4)	(189	4)	(190	3)	(191	12)	(193	13)
(194	3)	(195	15)	(196	3)	(197	4)	(202	4)
(203	3)	(205	4)	(207	24)	(208	6)	(209	6)
(210	4)	(211	71)	(212	11)	(213	7)	(218	4)
(219	6)	(220	91)	(221	17)	(222	8)	(225	39)
(226	8)	(227	18)	(228	3)	(233	3)	(234	6)
(237	10)	(238	3)	(241	4)	(242	4)	(243	3)
(255	4)	(268	4)	(269	4)	(274	4)	(277	3)
(283	8)	(284	4)	(285	8)	(298	18)	(299	171)
(300	50)	(301	25)	(302	5)	(313	5)	(314	18)
(315	149)	(316	42)	(317	22)	(318	4)	(329	4)
(343	6)	(355	3)	(356	11)	(357	6)	(358	8)
(359	25)	(360	8)	(361	4)	(372	3)	(373	6)
(374	3)	(385	5)	(386	34)	(387	121)	(388	49)
(389	26)	(390	7)	(417	5)	(451	5)	(461	3)
(462	9)	(463	4)	(550	3)				

NAME:13C\_2562.2\_1313EC07

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:256001-11-1

RI:2562

RT:15.693

NUM PEAKS: 136

( 71	8)	( 72	18)	( 73	1000)	( 74	92)	( 75	88)
( 76	8)	( 77	10)	( 84	3)	( 85	21)	( 86	7)
( 87	9)	( 88	5)	( 89	39)	( 90	13)	( 91	6)
( 98	3)	(100	4)	(101	9)	(102	12)	(103	40)

116

(104	98)	(105	20)	(106	6)	(107	3)	(114	3)
(115	10)	(116	18)	(117	9)	(118	15)	(119	24)
(120	5)	(121	5)	(129	3)	(130	5)	(131	20)
(132	72)	(133	62)	(134	30)	(135	16)	(136	3)
(137	5)	(144	3)	(145	10)	(146	11)	(147	133)
(148	24)	(150	5)	(151	5)	(158	4)	(160	6)
(161	29)	(162	6)	(163	6)	(164	3)	(165	3)
(173	11)	(174	7)	(175	4)	(176	12)	(177	5)
(181	6)	(183	3)	(188	3)	(189	4)	(190	3)
(191	15)	(192	15)	(193	10)	(194	3)	(195	6)
(203	5)	(204	5)	(205	4)	(206	25)	(207	17)
(208	5)	(209	3)	(211	37)	(212	6)	(213	3)
(218	4)	(219	6)	(220	38)	(221	9)	(222	6)
(225	11)	(227	8)	(232	4)	(233	4)	(234	3)
(235	4)	(243	3)	(247	3)	(248	3)	(249	3)
(250	3)	(251	6)	(255	5)	(264	5)	(265	10)
(266	5)	(283	5)	(284	3)	(285	5)	(298	10)
(299	89)	(300	28)	(301	12)	(313	3)	(314	7)
(315	41)	(316	12)	(317	6)	(329	4)	(331	3)
(336	4)	(343	6)	(344	3)	(358	8)	(359	34)
(360	11)	(361	5)	(372	3)	(373	4)	(385	4)
(386	33)	(387	116)	(388	51)	(389	24)	(390	6)
(403	3)	(474	6)	(475	16)	(476	8)	(477	5)
(478	3)								

NAME:13C\_2579.9\_1313EC07\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:258001-11-1

RI:2580

RT:15.787

NUM PEAKS: 335

( 70	29)	( 71	30)	( 72	214)	( 73	1000)	( 74	332)
( 75	309)	( 76	39)	( 77	31)	( 78	6)	( 79	8)
( 80	6)	( 82	7)	( 83	27)	( 84	13)	( 85	68)
( 86	31)	( 87	155)	( 88	55)	( 89	137)	( 90	45)
( 91	15)	( 92	8)	( 93	7)	( 94	6)	( 96	7)
( 98	32)	( 99	11)	(100	49)	(101	31)	(102	121)
(103	171)	(104	352)	(105	49)	(106	19)	(109	6)
(111	8)	(113	11)	(114	8)	(115	36)	(116	22)
(117	59)	(118	109)	(119	135)	(120	22)	(121	6)
(122	5)	(124	6)	(125	7)	(126	3)	(128	15)
(129	12)	(130	49)	(131	51)	(132	492)	(133	179)
(134	136)	(135	31)	(136	5)	(137	4)	(138	7)
(139	7)	(141	7)	(142	6)	(143	13)	(144	12)
(145	41)	(146	19)	(147	420)	(148	106)	(149	73)
(150	24)	(151	10)	(152	7)	(153	6)	(154	3)
(156	10)	(157	6)	(158	11)	(159	10)	(160	24)
(161	17)	(162	16)	(163	15)	(164	9)	(165	8)
(167	5)	(168	6)	(169	5)	(170	5)	(171	4)
(172	8)	(173	8)	(174	6)	(175	11)	(176	8)
(177	24)	(178	13)	(179	6)	(180	3)	(181	4)
(183	5)	(184	3)	(185	4)	(186	4)	(187	6)
(188	6)	(190	8)	(191	9)	(192	22)	(193	16)
(194	6)	(195	6)	(196	6)	(197	4)	(198	5)
(199	4)	(200	3)	(201	3)	(202	8)	(203	4)
(204	3)	(205	9)	(206	147)	(207	139)	(208	29)
(209	13)	(210	5)	(221	9)	(222	35)	(223	9)
(224	11)	(226	7)	(229	5)	(231	4)	(232	3)
(233	3)	(234	12)	(235	15)	(236	5)	(237	7)
(238	7)	(239	5)	(240	11)	(241	6)	(242	7)

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(243	4)	(244	3)	(245	4)	(246	8)	(247	4)
(249	4)	(250	4)	(252	20)	(253	43)	(254	8)
(256	4)	(260	4)	(262	4)	(265	5)	(266	7)
(267	31)	(268	15)	(269	7)	(270	5)	(271	4)
(272	4)	(275	3)	(279	6)	(280	9)	(281	5)
(282	8)	(283	6)	(284	3)	(285	4)	(290	3)
(292	7)	(294	4)	(295	4)	(296	8)	(297	24)
(298	11)	(300	5)	(301	4)	(302	4)	(303	3)
(305	4)	(306	5)	(307	3)	(309	9)	(310	7)
(311	7)	(312	6)	(313	3)	(314	6)	(315	5)
(316	8)	(317	5)	(318	4)	(319	3)	(320	4)
(321	3)	(322	5)	(325	11)	(326	10)	(327	14)
(328	3)	(329	4)	(331	7)	(332	6)	(334	5)
(337	5)	(338	4)	(340	7)	(344	6)	(345	6)
(347	5)	(348	6)	(353	3)	(355	8)	(356	6)
(357	5)	(360	4)	(361	7)	(371	6)	(373	5)
(374	4)	(375	5)	(378	4)	(381	7)	(382	5)
(383	4)	(384	5)	(385	15)	(386	27)	(387	88)
(388	29)	(389	9)	(390	4)	(391	4)	(395	6)
(396	6)	(397	4)	(398	7)	(399	7)	(400	8)
(401	15)	(402	7)	(403	10)	(406	4)	(408	4)
(409	3)	(410	5)	(412	4)	(415	7)	(419	5)
(420	5)	(422	3)	(423	5)	(424	5)	(429	4)
(430	3)	(431	7)	(432	4)	(438	4)	(439	6)
(440	4)	(441	3)	(443	4)	(444	4)	(446	4)
(447	4)	(453	3)	(454	4)	(455	5)	(456	5)
(458	5)	(459	6)	(460	4)	(461	4)	(462	5)
(463	5)	(464	6)	(465	5)	(466	3)	(467	3)
(472	5)	(473	6)	(474	4)	(475	9)	(476	12)
(477	9)	(478	6)	(479	4)	(483	4)	(484	4)
(485	6)	(486	4)	(488	5)	(491	4)	(492	6)
(493	6)	(496	3)	(497	4)	(502	4)	(503	5)
(506	5)	(508	3)	(509	5)	(512	4)	(517	3)
(522	7)	(525	4)	(526	4)	(528	5)	(531	4)
(536	3)	(539	3)	(540	3)	(541	7)	(542	3)
(544	5)	(546	4)	(547	4)	(548	3)	(550	3)
(551	3)	(552	4)	(555	3)	(558	5)	(561	4)
(564	3)	(572	4)	(584	3)	(590	3)	(591	3)

NAME:13C\_2390.1\_1313EC07\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:239001-11-1

RI:2390

RT:14.779

NUM PEAKS: 108

( 70	5)	( 71	9)	( 73	1000)	( 74	90)	( 75	102)
( 76	7)	( 77	11)	( 84	3)	( 85	8)	( 86	16)
( 87	8)	( 88	4)	( 89	7)	( 90	4)	( 99	3)
(100	3)	(101	5)	(102	9)	(103	28)	(104	29)
(105	10)	(107	3)	(113	3)	(114	5)	(115	15)
(116	15)	(117	8)	(118	14)	(119	15)	(121	3)
(130	4)	(131	22)	(132	113)	(133	65)	(134	13)
(135	15)	(137	5)	(145	5)	(146	13)	(147	149)
(148	26)	(149	22)	(150	3)	(151	5)	(160	10)
(161	7)	(164	3)	(174	10)	(175	3)	(176	3)
(177	3)	(181	6)	(189	5)	(191	26)	(192	37)
(193	16)	(194	4)	(195	6)	(205	7)	(206	163)
(207	40)	(208	15)	(209	3)	(211	41)	(212	7)
(213	4)	(219	3)	(220	45)	(221	11)	(222	5)
(225	9)	(226	3)	(227	8)	(235	3)	(243	3)

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(247	5)	(248	6)	(249	3)	(255	5)	(271	4)
(276	6)	(277	13)	(278	3)	(283	4)	(285	5)
(298	11)	(299	98)	(300	28)	(301	13)	(302	3)
(308	4)	(314	6)	(315	28)	(316	8)	(317	4)
(351	6)	(358	6)	(359	26)	(360	8)	(361	4)
(372	5)	(373	17)	(374	6)	(386	24)	(387	82)
(388	35)	(389	18)	(390	5)				

NAME:13C\_2347.2\_1313EC07\_Glucose-6-phosphate methoxyamine {BP} (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:235002-11-1

RI:2347

RT:14.551

NUM PEAKS: 96

( 70	5)	( 71	10)	( 72	16)	( 73	1000)	( 74	89)
( 75	79)	( 76	5)	( 85	8)	( 86	5)	( 87	8)
( 88	3)	( 89	49)	( 90	9)	(101	13)	(102	12)
(104	43)	(107	3)	(115	8)	(116	11)	(118	17)
(119	12)	(120	3)	(121	4)	(131	17)	(132	73)
(133	70)	(134	18)	(135	15)	(137	6)	(145	4)
(146	9)	(147	114)	(148	19)	(149	13)	(151	6)
(158	3)	(160	4)	(161	33)	(162	40)	(163	15)
(164	3)	(173	3)	(174	5)	(181	7)	(192	7)
(193	10)	(194	3)	(195	8)	(197	3)	(207	15)
(208	3)	(209	3)	(211	46)	(212	8)	(213	4)
(220	30)	(225	13)	(226	3)	(227	10)	(233	4)
(234	5)	(235	5)	(243	4)	(248	3)	(251	6)
(255	5)	(283	4)	(285	4)	(298	12)	(299	105)
(300	32)	(301	15)	(302	3)	(313	3)	(314	8)
(315	46)	(316	14)	(317	7)	(331	4)	(343	5)
(344	3)	(358	8)	(359	35)	(360	11)	(361	5)
(373	4)	(385	3)	(386	32)	(387	116)	(388	49)
(389	26)	(390	7)	(474	4)	(475	12)	(476	6)
(477	3)								

NAME:13C\_2313.4\_1313EC07\_Galactose-6-phosphate methoxyamine (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:232001-11-1

RI:2313

RT:14.372

NUM PEAKS: 108

( 70	5)	( 71	5)	( 72	17)	( 73	1000)	( 74	90)
( 75	91)	( 76	5)	( 77	9)	( 86	9)	( 87	11)
( 88	5)	( 89	37)	( 90	8)	( 91	4)	(100	3)
(101	14)	(102	12)	(103	48)	(105	23)	(106	4)
(107	3)	(115	10)	(116	17)	(117	9)	(118	16)
(119	14)	(121	4)	(129	3)	(130	6)	(131	20)
(132	72)	(133	66)	(134	16)	(135	15)	(137	6)
(144	4)	(145	7)	(146	11)	(147	144)	(148	24)
(149	16)	(151	6)	(159	3)	(160	5)	(161	30)
(162	61)	(163	14)	(164	4)	(173	4)	(174	5)
(175	3)	(176	5)	(177	4)	(181	7)	(189	3)
(190	3)	(191	14)	(192	9)	(193	11)	(195	8)
(203	3)	(204	3)	(205	4)	(206	12)	(207	19)
(208	5)	(209	3)	(211	42)	(212	7)	(213	4)
(218	6)	(219	8)	(225	12)	(226	3)	(227	10)
(232	3)	(233	4)	(234	6)	(235	5)	(248	3)
(249	3)	(251	4)	(255	5)	(283	4)	(285	4)
(298	9)	(299	89)	(300	26)	(301	13)	(302	3)
(331	6)	(336	6)	(343	6)	(358	7)	(359	32)

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(360 10) (361 5) (373 3) (385 3) (386 27)  
 (387 101) (388 42) (389 23) (390 6) (474 4)  
 (475 11) (476 5) (477 3)

NAME:13C\_2311.9\_1313EC07\_Fructose-6-phosphate methoxyamine (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:232002-11-1

RI:2312

RT:14.363

NUM PEAKS: 135

( 70 4) ( 71 8) ( 72 12) ( 73 1000) ( 74 93)  
 ( 75 16) ( 77 5) ( 85 27) ( 86 5) ( 89 36)  
 ( 90 15) ( 91 6) ( 98 3) (101 4) (102 5)  
 (103 37) (104 122) (105 12) (106 7) (114 3)  
 (115 7) (116 18) (117 8) (118 12) (119 33)  
 (120 7) (129 4) (130 4) (131 19) (132 87)  
 (133 47) (134 30) (135 14) (137 6) (142 3)  
 (145 9) (146 5) (147 163) (148 27) (149 18)  
 (150 3) (151 5) (158 3) (159 4) (160 6)  
 (173 9) (174 3) (175 3) (176 7) (177 3)  
 (181 8) (183 3) (186 4) (188 3) (189 4)  
 (191 6) (192 11) (193 9) (195 8) (203 4)  
 (204 3) (205 3) (206 14) (207 16) (208 6)  
 (209 3) (211 52) (212 10) (213 5) (217 3)  
 (218 3) (219 9) (220 177) (221 39) (222 17)  
 (223 4) (225 15) (226 4) (227 21) (228 4)  
 (233 3) (237 3) (248 4) (249 3) (255 5)  
 (260 3) (261 4) (262 3) (263 3) (264 5)  
 (265 10) (266 4) (267 3) (274 3) (276 3)  
 (283 3) (285 5) (297 3) (298 10) (299 86)  
 (300 31) (301 15) (302 4) (306 3) (307 3)  
 (308 3) (309 3) (313 3) (314 28) (315 274)  
 (316 79) (317 41) (318 8) (319 3) (322 3)  
 (323 3) (329 4) (343 6) (344 3) (345 3)  
 (358 5) (359 19) (360 7) (361 4) (362 3)  
 (372 3) (373 7) (374 5) (402 4) (403 11)  
 (404 5) (461 12) (462 30) (463 14) (464 6)

NAME:13C\_2257.9\_1313EC07

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:226001-11-1

RI:2258

RT:14.076

NUM PEAKS: 138

( 70 7) ( 71 10) ( 72 31) ( 73 1000) ( 74 113)  
 ( 75 105) ( 76 8) ( 84 5) ( 85 15) ( 86 9)  
 ( 87 25) ( 88 20) ( 89 245) ( 90 21) ( 98 3)  
 ( 99 3) (100 9) (101 16) (102 13) (103 20)  
 (104 187) (105 17) (106 5) (113 4) (114 5)  
 (115 9) (116 12) (118 12) (119 53) (130 8)  
 (131 25) (132 24) (133 39) (134 10) (142 4)  
 (144 6) (145 19) (146 20) (147 228) (148 44)  
 (149 22) (156 3) (157 5) (158 4) (159 7)  
 (160 8) (161 10) (163 5) (171 3) (172 6)  
 (173 14) (174 5) (175 8) (176 12) (177 7)  
 (178 5) (179 26) (180 3) (186 5) (187 6)  
 (188 9) (189 7) (190 3) (191 19) (192 16)  
 (193 7) (202 4) (203 5) (204 6) (205 5)  
 (207 25) (208 28) (209 4) (214 3) (218 3)  
 (219 7) (220 78) (221 20) (222 6) (232 4)

120

(233	12)	(246	3)	(247	8)	(248	3)	(251	3)
(259	3)	(260	4)	(261	7)	(262	6)	(263	4)
(265	6)	(266	3)	(274	3)	(275	4)	(276	6)
(277	3)	(278	3)	(279	7)	(280	3)	(291	3)
(292	3)	(293	3)	(294	4)	(296	3)	(304	3)
(305	3)	(306	3)	(307	4)	(309	3)	(310	7)
(334	5)	(335	14)	(336	7)	(337	3)	(350	3)
(351	6)	(352	5)	(378	4)	(379	3)	(380	8)
(381	9)	(382	23)	(383	7)	(410	3)	(411	4)
(441	3)	(442	4)	(452	3)	(453	8)	(454	4)
(468	4)	(483	4)	(484	3)	(558	5)	(559	3)
(560	3)	(561	6)	(562	3)				

NAME:13C\_2294.1\_1313EC07\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:230001-11-1

RI:2294

RT:14.269

NUM PEAKS: 188

( 70	7)	( 71	5)	( 73	758)	( 74	78)	( 75	66)
( 80	4)	( 82	5)	( 86	7)	( 90	24)	( 94	9)
( 97	6)	( 99	15)	(103	62)	(104	320)	(105	34)
(107	9)	(110	12)	(112	9)	(113	4)	(115	21)
(116	18)	(117	21)	(118	21)	(125	5)	(130	14)
(132	78)	(133	56)	(135	12)	(136	7)	(141	5)
(143	11)	(144	8)	(146	31)	(148	24)	(149	20)
(152	7)	(153	5)	(156	8)	(157	24)	(161	11)
(162	11)	(164	12)	(166	8)	(168	13)	(172	7)
(173	6)	(174	15)	(176	7)	(179	12)	(183	6)
(184	9)	(185	9)	(187	11)	(188	6)	(191	31)
(192	54)	(193	9)	(195	14)	(196	6)	(197	9)
(198	8)	(199	8)	(200	9)	(204	8)	(205	40)
(206	1000)	(207	122)	(208	63)	(213	6)	(214	6)
(215	12)	(217	22)	(218	7)	(220	50)	(221	23)
(222	41)	(223	8)	(232	6)	(234	9)	(236	15)
(237	15)	(243	7)	(244	13)	(246	5)	(247	7)
(252	7)	(253	8)	(257	6)	(259	12)	(260	15)
(263	14)	(264	10)	(268	12)	(269	16)	(271	10)
(272	17)	(278	6)	(292	10)	(302	6)	(308	7)
(309	7)	(317	14)	(323	10)	(324	10)	(326	10)
(330	7)	(332	12)	(333	6)	(339	15)	(340	15)
(341	39)	(343	12)	(345	9)	(346	8)	(353	12)
(364	14)	(365	13)	(366	12)	(367	20)	(368	9)
(371	12)	(376	14)	(378	12)	(379	13)	(383	13)
(384	10)	(389	9)	(390	5)	(391	12)	(394	8)
(395	8)	(402	18)	(408	9)	(410	10)	(411	7)
(415	7)	(421	13)	(426	8)	(430	10)	(443	13)
(447	24)	(448	9)	(449	10)	(453	16)	(454	12)
(458	9)	(459	12)	(461	11)	(471	8)	(477	9)
(480	18)	(483	6)	(484	13)	(488	10)	(489	8)
(491	9)	(493	13)	(494	8)	(499	12)	(502	10)
(503	15)	(504	7)	(505	8)	(509	12)	(510	12)
(513	18)	(514	14)	(515	17)	(524	8)	(528	12)
(529	9)	(532	8)	(533	13)	(548	14)	(549	16)
(553	7)	(555	16)	(559	5)	(560	6)	(563	7)
(566	7)	(569	12)	(571	13)	(575	7)	(578	4)
(580	6)	(590	7)	(591	8)				

NAME:13C\_2285.3\_1313EC07\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:228001-11-1

RI:2285

RT:14.222

NUM PEAKS: 106

( 71	7)	( 72	20)	( 73	1000)	( 74	95)	( 75	145)
( 76	9)	( 77	5)	( 85	6)	( 86	9)	( 87	12)
( 88	4)	( 89	39)	( 90	15)	(100	4)	(101	17)
(102	15)	(103	51)	(104	36)	(105	26)	(106	3)
(116	14)	(117	10)	(118	133)	(119	330)	(120	29)
(121	13)	(130	5)	(131	16)	(132	62)	(133	44)
(134	15)	(135	5)	(144	4)	(145	9)	(146	25)
(147	132)	(148	25)	(149	18)	(160	8)	(161	98)
(162	120)	(163	60)	(164	10)	(165	3)	(173	5)
(174	5)	(176	6)	(177	6)	(190	3)	(191	16)
(192	9)	(193	11)	(203	3)	(204	4)	(206	6)
(207	9)	(209	4)	(215	3)	(216	5)	(218	6)
(219	10)	(220	71)	(221	20)	(222	9)	(233	4)
(234	8)	(235	16)	(236	7)	(237	15)	(238	3)
(248	5)	(251	13)	(252	3)	(253	13)	(262	5)
(263	3)	(264	3)	(265	4)	(274	3)	(278	4)
(280	5)	(281	4)	(294	4)	(296	10)	(297	82)
(298	16)	(306	4)	(307	3)	(308	4)	(309	3)
(310	4)	(323	10)	(324	4)	(325	10)	(326	3)
(327	3)	(333	3)	(334	4)	(352	3)	(368	3)
(412	6)	(413	25)	(414	9)	(415	4)	(441	3)
(513	3)								

NAME:13C\_1396.1\_1313EC11\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:140003-11-1

RI:1396

RT: 7.541

NUM PEAKS: 66

( 70	5)	( 71	5)	( 72	21)	( 73	1000)	( 74	85)
( 75	322)	( 76	10)	( 77	10)	( 84	1)	( 85	6)
( 86	2)	( 91	12)	( 99	2)	(103	50)	(104	8)
(105	6)	(110	1)	(112	3)	(117	13)	(118	192)
(119	660)	(120	59)	(121	21)	(126	2)	(133	129)
(134	15)	(135	14)	(136	2)	(137	2)	(144	3)
(146	9)	(149	115)	(150	15)	(161	2)	(163	4)
(176	9)	(177	11)	(178	4)	(191	2)	(192	2)
(193	3)	(200	4)	(207	13)	(208	3)	(209	2)
(211	1)	(216	2)	(235	3)	(236	10)	(237	134)
(238	23)	(239	9)	(242	1)	(249	1)	(250	24)
(251	3)	(252	3)	(268	6)	(288	1)	(308	7)
(309	89)	(310	24)	(311	14)	(312	2)	(340	7)
(341	2)								

NAME:13C\_1475.5\_1313EC07\_Citramalic acid (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:148001-11-1

RI:1476

RT: 8.482

NUM PEAKS: 94

( 70	7)	( 71	15)	( 72	90)	( 73	1000)	( 74	95)
( 75	209)	( 76	21)	( 77	7)	( 86	3)	( 87	10)
( 88	5)	( 89	37)	(100	11)	(101	9)	(102	18)
(103	14)	(104	5)	(116	5)	(117	16)	(118	125)
(119	15)	(120	4)	(131	28)	(132	10)	(133	76)
(134	11)	(135	10)	(136	1)	(137	1)	(146	9)

122

(147	368)	(148	69)	(149	76)	(150	10)	(151	7)
(152	1)	(160	4)	(161	19)	(162	2)	(163	28)
(164	4)	(165	2)	(174	4)	(175	5)	(176	3)
(178	1)	(190	22)	(191	9)	(192	21)	(193	8)
(194	2)	(206	31)	(207	11)	(208	3)	(211	2)
(218	1)	(219	8)	(221	32)	(222	7)	(223	3)
(224	1)	(227	2)	(229	1)	(234	26)	(235	35)
(236	18)	(237	5)	(238	1)	(247	1)	(250	7)
(251	136)	(252	23)	(253	11)	(254	1)	(263	2)
(264	32)	(265	5)	(266	4)	(280	3)	(293	1)
(299	3)	(301	1)	(308	2)	(309	4)	(310	1)
(322	1)	(324	1)	(325	15)	(326	6)	(337	2)
(338	1)	(353	1)	(354	10)	(355	3)		

NAME:13C\_1735.8\_1313EC07\_Glycerol-2-phosphate (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:174002-11-1

RI:1736

RT: 10.586

NUM PEAKS: 421

( 70	8)	( 71	21)	( 72	39)	( 73	1000)	( 74	110)
( 75	219)	( 76	14)	( 77	39)	( 78	3)	( 79	13)
( 80	14)	( 81	10)	( 82	19)	( 83	10)	( 84	26)
( 85	11)	( 86	1)	( 87	155)	( 88	35)	( 89	31)
( 90	8)	( 91	27)	( 92	8)	( 93	5)	( 94	7)
( 95	3)	( 96	4)	( 98	16)	( 99	11)	(100	28)
(101	25)	(102	49)	(103	149)	(105	26)	(106	11)
(107	16)	(108	3)	(109	10)	(111	10)	(112	10)
(113	14)	(114	6)	(115	51)	(116	20)	(117	29)
(118	82)	(121	25)	(124	15)	(127	24)	(128	34)
(129	33)	(130	24)	(131	47)	(132	136)	(133	81)
(134	15)	(135	20)	(136	5)	(137	14)	(138	8)
(139	6)	(141	49)	(142	12)	(144	12)	(146	15)
(147	185)	(148	5)	(149	12)	(151	24)	(152	34)
(153	19)	(154	4)	(155	27)	(156	19)	(157	61)
(158	2)	(159	23)	(160	11)	(162	13)	(165	4)
(166	10)	(167	2)	(168	2)	(169	2)	(170	9)
(171	7)	(172	7)	(174	1)	(175	435)	(176	28)
(177	42)	(178	5)	(179	22)	(180	95)	(181	46)
(182	16)	(183	16)	(184	15)	(185	15)	(186	19)
(187	4)	(189	25)	(190	73)	(191	3)	(192	14)
(193	23)	(194	8)	(195	12)	(196	14)	(197	18)
(198	29)	(199	8)	(201	15)	(202	5)	(203	25)
(205	1)	(210	3)	(211	227)	(212	41)	(213	31)
(214	9)	(215	6)	(216	9)	(217	18)	(218	21)
(223	14)	(224	3)	(225	8)	(227	38)	(228	2)
(229	13)	(230	1)	(231	76)	(232	24)	(234	2)
(235	2)	(236	5)	(238	14)	(239	4)	(240	6)
(242	20)	(243	294)	(244	54)	(245	38)	(246	11)
(247	3)	(249	11)	(251	1)	(252	9)	(253	9)
(255	7)	(256	6)	(257	9)	(258	3)	(259	17)
(260	16)	(261	8)	(263	5)	(265	10)	(266	3)
(267	9)	(268	14)	(269	83)	(270	22)	(271	8)
(272	3)	(273	3)	(274	12)	(275	14)	(276	12)
(277	13)	(280	9)	(282	6)	(283	26)	(284	17)
(285	32)	(286	12)	(287	12)	(288	6)	(291	4)
(294	8)	(295	8)	(296	7)	(297	5)	(298	19)
(299	173)	(300	60)	(301	36)	(302	8)	(303	5)
(304	6)	(306	1)	(308	32)	(309	24)	(311	3)
(312	7)	(313	9)	(314	14)	(315	36)	(316	14)



123

(318	7)	(319	6)	(320	9)	(321	25)	(322	4)
(326	8)	(329	12)	(330	3)	(331	12)	(332	9)
(333	8)	(334	7)	(337	9)	(338	9)	(339	9)
(340	9)	(341	4)	(343	8)	(344	2)	(345	5)
(346	9)	(347	12)	(348	22)	(349	8)	(351	13)
(352	9)	(353	8)	(355	8)	(356	7)	(357	9)
(358	5)	(359	8)	(360	10)	(361	5)	(362	5)
(363	12)	(364	3)	(365	4)	(370	11)	(371	3)
(372	13)	(373	21)	(374	15)	(375	21)	(376	13)
(377	12)	(378	18)	(379	3)	(380	15)	(381	5)
(384	5)	(385	15)	(386	7)	(387	6)	(388	7)
(389	27)	(390	18)	(391	4)	(392	10)	(393	9)
(394	10)	(395	9)	(396	12)	(397	6)	(398	3)
(399	14)	(400	9)	(401	17)	(402	1)	(403	6)
(404	13)	(405	6)	(407	7)	(408	3)	(409	4)
(411	12)	(414	2)	(415	7)	(416	15)	(417	11)
(418	8)	(419	4)	(420	7)	(421	2)	(422	3)
(423	15)	(424	4)	(426	13)	(427	2)	(429	5)
(430	2)	(431	1)	(432	4)	(433	1)	(435	3)
(436	15)	(437	7)	(439	13)	(440	15)	(441	1)
(442	5)	(443	2)	(444	3)	(446	6)	(447	6)
(448	22)	(449	12)	(450	5)	(451	6)	(452	7)
(453	4)	(454	10)	(455	12)	(457	2)	(459	12)
(460	12)	(461	11)	(463	10)	(466	6)	(467	9)
(470	15)	(471	12)	(472	3)	(473	9)	(475	14)
(476	10)	(478	1)	(479	6)	(480	10)	(481	6)
(482	8)	(483	1)	(484	9)	(485	13)	(486	2)
(487	5)	(488	6)	(489	4)	(491	10)	(492	6)
(493	10)	(494	8)	(495	9)	(496	5)	(498	8)
(499	9)	(500	6)	(501	8)	(502	2)	(503	7)
(504	9)	(505	2)	(507	9)	(508	5)	(509	23)
(510	9)	(512	7)	(513	3)	(514	2)	(516	11)
(517	9)	(518	7)	(519	8)	(520	6)	(521	5)
(522	11)	(523	2)	(524	10)	(525	9)	(527	5)
(528	18)	(529	13)	(530	15)	(531	3)	(532	4)
(534	2)	(535	11)	(536	6)	(538	5)	(539	2)
(540	5)	(541	3)	(542	6)	(543	12)	(544	6)
(546	5)	(550	11)	(551	8)	(552	11)	(554	3)
(555	4)	(557	1)	(558	9)	(561	10)	(562	4)
(563	6)	(564	1)	(565	7)	(566	9)	(569	1)
(570	3)	(571	2)	(572	11)	(573	9)	(574	3)
(575	1)	(576	1)	(578	2)	(581	3)	(582	1)
(583	2)	(584	9)	(587	1)	(588	8)	(590	1)
(591	3)	(592	2)	(594	3)	(595	1)	(596	2)
(597	3)								

NAME:13C\_1755.8\_1313EC07

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:176003-11-1

RI:1756

RT: 10.758

NUM PEAKS: 124

( 70	30)	( 71	81)	( 72	51)	( 73	1000)	( 79	12)
( 80	5)	( 81	5)	( 84	11)	( 85	57)	( 86	17)
( 87	45)	( 91	4)	( 92	3)	( 93	6)	( 94	3)
( 97	10)	( 98	3)	( 99	39)	(101	125)	(102	20)
(103	15)	(108	2)	(109	2)	(112	5)	(113	14)
(114	5)	(115	26)	(117	20)	(121	1)	(122	1)
(125	2)	(126	7)	(127	10)	(130	4)	(131	56)
(133	62)	(134	9)	(135	5)	(140	2)	(142	5)

124

(143	18)	(147	245)	(148	47)	(149	22)	(156	2)
(157	4)	(158	16)	(159	21)	(161	7)	(170	3)
(171	10)	(174	12)	(175	50)	(176	9)	(184	6)
(185	7)	(186	5)	(187	7)	(199	3)	(200	9)
(201	4)	(206	19)	(214	5)	(216	5)	(217	16)
(230	5)	(242	4)	(243	15)	(244	6)	(245	4)
(246	4)	(250	1)	(256	11)	(257	69)	(258	282)
(259	63)	(260	23)	(261	4)	(262	3)	(272	2)
(273	9)	(274	45)	(275	9)	(276	4)	(287	9)
(288	4)	(289	3)	(290	3)	(291	1)	(301	2)
(308	1)	(309	1)	(315	1)	(317	3)	(331	6)
(332	6)	(333	8)	(334	5)	(337	2)	(347	3)
(360	5)	(361	21)	(362	79)	(363	23)	(364	10)
(369	1)	(370	1)	(376	7)	(377	9)	(378	3)
(387	1)	(388	1)	(418	1)	(443	2)	(455	1)
(466	1)	(489	2)	(506	1)	(513	1)	(558	1)
(573	1)	(584	1)	(589	1)	(592	1)		

NAME:13C\_1761.5\_1313EC07\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:176004-11-1

RI:1762

RT: 10.791

NUM PEAKS: 88

( 70	13)	( 73	1000)	( 83	4)	( 89	102)	( 90	22)
( 91	5)	( 98	5)	( 99	44)	(103	42)	(104	95)
(105	41)	(106	5)	(111	1)	(119	73)	(120	7)
(121	2)	(127	5)	(128	8)	(129	28)	(133	68)
(134	35)	(135	8)	(136	1)	(143	8)	(144	10)
(145	214)	(147	114)	(149	14)	(156	2)	(157	4)
(163	11)	(164	2)	(170	1)	(171	3)	(172	12)
(173	26)	(185	4)	(186	5)	(187	4)	(188	13)
(189	60)	(201	4)	(202	6)	(203	19)	(205	20)
(206	8)	(207	36)	(208	5)	(209	2)	(217	7)
(231	7)	(232	2)	(234	24)	(235	500)	(236	57)
(237	19)	(238	1)	(247	3)	(261	1)	(271	1)
(276	2)	(277	5)	(278	1)	(279	2)	(290	2)
(291	2)	(292	2)	(305	1)	(306	1)	(307	1)
(309	1)	(310	6)	(311	1)	(319	1)	(320	3)
(321	18)	(322	4)	(323	1)	(337	4)	(338	3)
(339	1)	(348	1)	(410	2)	(411	7)	(412	2)
(413	1)	(426	1)	(427	2)				

NAME:13C\_1796.3\_1313EC07\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:180001-11-1

RI:1796

RT: 11.063

NUM PEAKS: 145

( 70	21)	( 71	20)	( 72	35)	( 73	1000)	( 74	95)
( 75	235)	( 76	17)	( 77	12)	( 84	8)	( 85	17)
( 86	11)	( 87	38)	( 88	133)	( 89	79)	( 90	19)
( 91	6)	( 92	2)	( 98	9)	( 99	101)	(100	16)
(101	23)	(102	17)	(103	68)	(104	117)	(105	88)
(106	11)	(107	3)	(113	4)	(114	4)	(115	19)
(116	13)	(117	15)	(118	44)	(119	71)	(120	8)
(121	2)	(126	1)	(127	7)	(128	12)	(129	11)
(130	10)	(131	32)	(132	71)	(133	85)	(134	27)
(135	7)	(136	1)	(142	2)	(143	5)	(144	12)
(145	22)	(146	15)	(147	142)	(148	32)	(149	27)

125

(150	3)	(151	3)	(156	3)	(157	4)	(158	6)
(159	14)	(160	58)	(161	14)	(162	52)	(163	20)
(164	4)	(166	1)	(172	8)	(173	18)	(174	6)
(177	11)	(178	18)	(179	2)	(183	4)	(187	3)
(188	2)	(189	6)	(191	36)	(192	21)	(199	2)
(200	4)	(202	6)	(203	80)	(204	13)	(205	29)
(206	18)	(207	43)	(208	8)	(209	3)	(217	4)
(218	6)	(219	3)	(220	47)	(221	9)	(222	39)
(223	4)	(224	1)	(230	1)	(231	7)	(232	2)
(233	5)	(234	11)	(235	109)	(236	13)	(237	4)
(240	1)	(246	2)	(247	2)	(248	7)	(249	1)
(263	6)	(264	1)	(275	3)	(276	2)	(277	7)
(278	2)	(279	2)	(281	3)	(282	3)	(290	2)
(291	1)	(296	1)	(305	2)	(306	2)	(308	1)
(309	2)	(310	11)	(311	3)	(312	1)	(320	3)
(321	20)	(322	5)	(323	2)	(324	2)	(325	9)
(326	1)	(336	1)	(337	5)	(338	5)	(351	1)
(352	2)	(381	1)	(411	3)	(412	1)	(427	1)

NAME:13C\_3379.6\_1313EC07\_Lanosta-8,24-dien-3-beta-ol (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:338001-11-1

RI:3380

RT:19.444

NUM PEAKS: 303

( 70	50)	( 71	29)	( 72	235)	( 73	810)	( 74	1000)
( 75	516)	( 76	61)	( 77	21)	( 78	5)	( 79	6)
( 80	8)	( 81	9)	( 82	17)	( 83	91)	( 84	31)
( 85	144)	( 86	29)	( 87	250)	( 88	41)	( 89	135)
( 90	10)	( 91	23)	( 92	5)	( 93	5)	( 94	6)
( 95	8)	( 96	14)	( 97	19)	( 98	182)	( 99	28)
(100	176)	(101	38)	(102	289)	(103	33)	(104	53)
(105	8)	(106	5)	(107	5)	(109	7)	(110	9)
(111	24)	(112	25)	(113	199)	(114	28)	(115	176)
(116	40)	(117	303)	(118	22)	(119	49)	(120	15)
(121	5)	(122	4)	(123	8)	(124	50)	(125	21)
(126	68)	(127	27)	(128	189)	(129	33)	(130	157)
(131	37)	(132	342)	(133	32)	(134	25)	(135	8)
(136	7)	(137	24)	(138	57)	(139	68)	(140	31)
(141	118)	(142	24)	(143	124)	(144	28)	(145	133)
(146	17)	(147	67)	(148	13)	(149	10)	(150	7)
(151	8)	(152	39)	(153	36)	(154	74)	(155	35)
(156	130)	(157	28)	(158	118)	(159	20)	(160	77)
(161	8)	(162	40)	(163	10)	(164	16)	(165	18)
(166	13)	(167	31)	(168	22)	(169	64)	(170	27)
(171	111)	(172	41)	(173	98)	(174	15)	(175	48)
(176	8)	(177	22)	(178	17)	(179	6)	(180	11)
(181	10)	(182	25)	(183	16)	(184	55)	(185	25)
(186	90)	(187	25)	(188	63)	(189	7)	(190	29)
(191	6)	(192	12)	(193	11)	(194	3)	(195	9)
(196	7)	(197	22)	(198	14)	(199	55)	(200	26)
(201	104)	(202	23)	(203	80)	(204	15)	(205	31)
(206	5)	(207	6)	(208	7)	(209	3)	(210	5)
(211	8)	(212	17)	(213	16)	(214	42)	(215	15)
(216	48)	(217	14)	(218	37)	(219	8)	(220	20)
(221	9)	(222	3)	(226	6)	(227	14)	(228	13)
(229	41)	(230	18)	(231	55)	(232	7)	(233	18)
(234	3)	(235	10)	(238	3)	(239	4)	(240	6)
(241	6)	(242	14)	(243	15)	(244	55)	(245	13)
(246	47)	(247	6)	(248	9)	(249	3)	(254	4)

126

(255	5)	(256	5)	(257	15)	(258	20)	(259	79)
(260	12)	(261	24)	(262	6)	(263	5)	(264	3)
(266	4)	(270	4)	(272	10)	(273	8)	(274	35)
(275	5)	(276	21)	(277	5)	(278	3)	(285	5)
(286	5)	(287	10)	(288	6)	(289	17)	(290	8)
(291	12)	(292	10)	(293	6)	(298	3)	(300	4)
(301	6)	(302	12)	(303	7)	(304	11)	(305	5)
(306	6)	(307	5)	(314	3)	(315	3)	(316	5)
(317	8)	(318	6)	(319	10)	(320	3)	(321	6)
(327	3)	(328	3)	(330	3)	(331	4)	(332	9)
(333	4)	(334	14)	(336	3)	(338	3)	(341	3)
(344	3)	(345	3)	(346	6)	(347	11)	(348	4)
(349	7)	(350	5)	(351	4)	(352	4)	(355	3)
(362	7)	(363	3)	(364	5)	(367	3)	(370	3)
(371	4)	(374	3)	(375	4)	(376	7)	(377	7)
(379	4)	(380	4)	(386	4)	(387	4)	(388	3)
(389	3)	(391	3)	(392	3)	(396	3)	(405	3)
(406	3)	(413	3)	(414	3)	(419	7)	(420	19)
(421	53)	(422	149)	(423	29)	(429	3)	(433	3)
(436	3)	(437	5)	(441	3)	(445	4)	(455	3)
(457	3)	(461	3)	(466	3)	(471	3)	(477	3)
(486	3)	(492	4)	(498	3)	(506	3)	(510	8)
(511	17)	(512	37)	(513	20)	(514	6)	(516	3)
(518	3)	(519	5)	(525	4)	(526	10)	(527	16)
(528	36)	(529	16)	(530	4)	(532	3)	(535	3)
(543	4)	(549	3)	(563	3)				

NAME:13C\_3079.3\_1313EC07

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:308001-11-1

RI:3079

RT:18.190

NUM PEAKS: 175

( 70	12)	( 71	14)	( 72	40)	( 73	1000)	( 74	96)
( 75	112)	( 76	8)	( 77	12)	( 83	5)	( 84	8)
( 85	10)	( 86	23)	( 87	11)	( 88	6)	( 89	7)
( 90	4)	( 91	4)	( 96	5)	( 97	3)	( 98	7)
( 99	6)	(100	11)	(101	10)	(102	22)	(103	28)
(104	9)	(105	7)	(107	3)	(111	6)	(112	25)
(113	6)	(114	5)	(115	13)	(116	15)	(117	15)
(118	12)	(119	13)	(121	5)	(123	3)	(124	7)
(125	3)	(126	4)	(129	10)	(130	6)	(131	24)
(132	63)	(133	82)	(134	13)	(135	21)	(136	3)
(137	10)	(138	4)	(139	15)	(140	71)	(141	66)
(142	3)	(143	3)	(144	24)	(145	15)	(146	28)
(147	154)	(148	26)	(149	21)	(150	3)	(151	8)
(152	4)	(153	6)	(154	9)	(155	7)	(158	11)
(159	4)	(160	5)	(161	6)	(162	3)	(165	3)
(167	7)	(168	6)	(169	12)	(170	34)	(172	4)
(173	21)	(174	418)	(175	42)	(176	41)	(177	4)
(179	3)	(180	3)	(181	18)	(182	7)	(183	10)
(184	3)	(189	6)	(190	3)	(191	10)	(192	3)
(193	10)	(194	4)	(195	18)	(196	9)	(197	22)
(198	5)	(199	4)	(205	3)	(206	3)	(207	14)
(208	4)	(209	5)	(210	8)	(211	114)	(212	32)
(213	36)	(214	5)	(218	12)	(219	5)	(220	16)
(222	3)	(223	4)	(224	9)	(225	20)	(226	7)
(227	25)	(228	6)	(229	3)	(233	7)	(234	123)
(235	22)	(236	10)	(240	6)	(241	17)	(242	9)
(243	11)	(247	13)	(248	43)	(249	10)	(250	4)

127

(255	7)	(256	7)	(257	15)	(258	3)	(262	9)
(263	65)	(264	16)	(265	6)	(269	5)	(270	7)
(271	7)	(272	19)	(273	3)	(283	4)	(284	3)
(285	8)	(286	3)	(298	8)	(299	76)	(300	24)
(301	12)	(302	3)	(312	4)	(313	8)	(314	25)
(315	214)	(316	66)	(317	30)	(318	6)	(329	3)
(373	3)	(374	8)	(385	3)	(386	19)	(387	11)
(388	6)	(389	3)	(403	5)	(404	15)	(405	3)

NAME:13C\_2679.5\_1313EC07

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:268001-11-1

RI:2680

RT:16.316

NUM PEAKS: 157

( 70	8)	( 71	9)	( 72	23)	( 73	1000)	( 74	91)
( 75	106)	( 76	7)	( 77	14)	( 83	3)	( 84	4)
( 85	8)	( 86	11)	( 87	9)	( 88	3)	( 89	10)
( 90	6)	( 91	4)	( 98	10)	( 99	3)	(100	3)
(101	6)	(102	9)	(103	24)	(104	30)	(105	9)
(106	3)	(107	4)	(113	5)	(114	4)	(115	21)
(116	9)	(117	7)	(118	7)	(119	18)	(121	5)
(129	5)	(130	5)	(131	17)	(132	72)	(133	69)
(134	13)	(135	19)	(136	3)	(137	9)	(139	4)
(140	4)	(141	23)	(144	16)	(145	9)	(146	21)
(147	156)	(148	27)	(149	23)	(150	4)	(151	9)
(158	3)	(159	4)	(160	12)	(161	14)	(162	3)
(163	3)	(165	3)	(174	9)	(175	3)	(176	3)
(177	3)	(178	9)	(179	4)	(181	11)	(182	3)
(183	4)	(188	4)	(189	11)	(190	3)	(191	12)
(192	16)	(193	13)	(194	3)	(195	12)	(196	3)
(197	4)	(202	4)	(203	4)	(205	7)	(206	28)
(207	27)	(208	6)	(209	5)	(210	5)	(211	72)
(212	12)	(213	7)	(217	3)	(218	43)	(219	15)
(220	33)	(225	32)	(226	9)	(227	23)	(228	4)
(233	9)	(234	64)	(235	14)	(236	6)	(242	5)
(243	6)	(248	3)	(255	3)	(256	4)	(260	3)
(262	8)	(263	3)	(269	3)	(276	5)	(277	12)
(278	3)	(283	6)	(284	4)	(285	12)	(286	4)
(298	16)	(299	133)	(300	42)	(301	20)	(302	5)
(313	5)	(314	19)	(315	147)	(316	45)	(317	22)
(318	4)	(328	4)	(329	20)	(330	6)	(331	4)
(343	3)	(344	5)	(351	3)	(358	6)	(359	11)
(360	4)	(372	3)	(373	5)	(374	3)	(375	5)
(386	5)	(387	17)	(388	8)	(389	5)	(429	3)
(445	3)	(446	10)	(447	20)	(448	9)	(449	5)
(450	3)	(518	3)						

NAME:13C\_1924.2\_1313EC07\_Mannitol (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:193002-11-1

RI:1924

RT:12.015

NUM PEAKS: 125

( 72	11)	( 73	1000)	( 74	89)	( 75	7)	( 87	26)
( 89	67)	( 90	32)	( 91	3)	(100	6)	(101	27)
(102	14)	(103	27)	(104	265)	(105	45)	(106	12)
(114	2)	(115	4)	(116	8)	(117	8)	(118	8)
(119	121)	(120	13)	(121	4)	(128	1)	(129	3)
(130	6)	(131	42)	(132	221)	(133	87)	(134	55)

128

(135	9)	(136	1)	(144	1)	(145	4)	(146	17)
(147	472)	(148	66)	(149	39)	(150	3)	(156	2)
(158	2)	(160	6)	(161	150)	(162	162)	(163	41)
(164	12)	(173	4)	(174	9)	(175	2)	(176	6)
(177	12)	(178	8)	(179	1)	(184	1)	(189	1)
(190	9)	(191	50)	(193	2)	(198	2)	(202	2)
(204	5)	(205	3)	(206	8)	(207	234)	(208	46)
(209	21)	(210	1)	(219	10)	(220	95)	(221	22)
(222	10)	(232	2)	(233	44)	(234	10)	(235	41)
(236	11)	(237	17)	(238	3)	(239	1)	(246	4)
(247	2)	(248	7)	(249	6)	(250	4)	(251	3)
(252	1)	(264	3)	(265	2)	(266	2)	(274	8)
(275	3)	(276	1)	(278	9)	(279	14)	(280	6)
(281	1)	(285	1)	(291	1)	(294	14)	(295	6)
(296	2)	(306	2)	(307	2)	(308	2)	(309	5)
(310	5)	(311	4)	(312	1)	(321	1)	(322	16)
(323	206)	(324	72)	(325	33)	(326	6)	(340	2)
(352	2)	(353	1)	(364	1)	(369	1)	(380	1)
(381	4)	(382	2)	(383	1)	(454	1)	(470	1)

NAME:13C\_1546.0\_1313EC07\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:154001-11-1

RI:1546

RT:9.114

NUM PEAKS: 256

( 70	14)	( 72	42)	( 73	1000)	( 74	277)	( 90	19)
(103	90)	(104	108)	(112	4)	(116	94)	(119	112)
(132	128)	(133	66)	(134	13)	(146	29)	(147	500)
(148	81)	(182	1)	(195	2)	(196	1)	(197	1)
(198	2)	(206	20)	(207	40)	(209	7)	(210	1)
(211	2)	(212	1)	(213	2)	(214	2)	(219	29)
(220	67)	(221	37)	(222	87)	(223	19)	(224	8)
(225	1)	(228	1)	(238	1)	(239	8)	(240	2)
(241	2)	(244	2)	(245	3)	(246	5)	(250	7)
(251	4)	(254	1)	(255	1)	(256	1)	(257	1)
(258	1)	(259	2)	(260	6)	(268	1)	(276	1)
(292	2)	(293	7)	(294	93)	(295	28)	(296	14)
(297	4)	(308	2)	(309	1)	(310	3)	(311	1)
(312	1)	(314	1)	(318	1)	(319	1)	(320	1)
(322	2)	(323	8)	(324	4)	(325	4)	(326	2)
(327	2)	(328	1)	(329	1)	(330	1)	(331	1)
(332	1)	(333	1)	(334	2)	(335	1)	(336	2)
(337	2)	(338	2)	(339	2)	(340	2)	(341	2)
(342	2)	(343	2)	(344	2)	(345	2)	(346	2)
(347	2)	(348	2)	(349	2)	(350	1)	(351	1)
(352	2)	(353	3)	(354	1)	(355	2)	(356	2)
(357	1)	(358	1)	(359	1)	(360	1)	(361	1)
(362	1)	(363	1)	(364	1)	(365	1)	(366	1)
(367	1)	(368	1)	(369	1)	(370	1)	(375	1)
(380	1)	(381	1)	(382	3)	(383	2)	(384	1)
(385	1)	(387	1)	(398	1)	(406	1)	(407	1)
(412	2)	(413	5)	(414	3)	(415	2)	(416	1)
(418	1)	(419	1)	(420	1)	(421	1)	(422	1)
(423	1)	(424	1)	(425	1)	(426	1)	(427	1)
(428	1)	(429	1)	(430	1)	(431	1)	(432	1)
(433	1)	(434	1)	(435	1)	(436	1)	(438	2)
(439	1)	(440	2)	(441	1)	(442	1)	(443	1)
(444	1)	(445	1)	(446	1)	(448	1)	(449	1)
(450	1)	(451	1)	(452	1)	(453	2)	(454	1)

129

(455	2)	(456	1)	(457	1)	(458	1)	(460	1)
(461	1)	(463	1)	(464	1)	(466	1)	(467	1)
(468	1)	(469	1)	(470	1)	(471	1)	(472	1)
(474	1)	(475	1)	(477	1)	(478	1)	(480	1)
(481	1)	(485	1)	(486	1)	(490	1)	(491	1)
(492	1)	(495	1)	(501	1)	(504	1)	(505	1)
(509	1)	(512	1)	(515	1)	(516	1)	(519	2)
(520	1)	(522	1)	(523	1)	(524	2)	(525	2)
(526	1)	(528	1)	(529	1)	(530	1)	(531	1)
(532	1)	(533	1)	(534	1)	(535	1)	(536	1)
(537	1)	(538	1)	(539	1)	(540	1)	(541	1)
(542	1)	(543	1)	(544	1)	(545	1)	(546	1)
(547	1)	(548	1)	(549	1)	(550	1)	(551	1)
(552	1)	(554	1)	(555	1)	(556	1)	(557	1)
(558	1)	(559	1)	(560	1)	(561	1)	(563	1)
(564	1)	(566	1)	(567	1)	(568	1)	(570	1)
(571	1)	(572	1)	(573	1)	(574	1)	(584	1)
(586	1)								

NAME:13C\_1281.6\_1313EC07\_Ethanolamine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1282 |RI:1282

CASNO:128002-11-1

RI:1282

RT:6.144

SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp

NUM PEAKS: 147

( 79	93)	( 87	108)	( 94	16)	(100	30)	(101	24)
(112	6)	(113	33)	(124	14)	(126	7)	(138	42)
(144	15)	(157	11)	(160	5)	(161	5)	(172	6)
(174	36)	(175	1000)	(176	177)	(180	30)	(183	4)
(190	1)	(198	5)	(202	3)	(203	11)	(204	29)
(212	6)	(217	9)	(222	2)	(231	9)	(233	4)
(242	15)	(244	26)	(245	13)	(252	15)	(260	6)
(262	26)	(263	15)	(264	19)	(276	8)	(277	4)
(279	20)	(281	42)	(282	13)	(284	28)	(287	5)
(291	12)	(296	10)	(298	27)	(306	24)	(307	6)
(309	3)	(313	30)	(322	15)	(324	2)	(328	22)
(333	6)	(335	40)	(336	41)	(343	16)	(344	5)
(346	1)	(347	13)	(349	17)	(354	27)	(355	18)
(360	19)	(361	34)	(362	15)	(363	10)	(364	9)
(368	1)	(369	26)	(372	13)	(374	20)	(376	41)
(388	14)	(393	16)	(398	11)	(399	15)	(401	3)
(402	7)	(405	16)	(406	6)	(408	9)	(409	17)
(410	61)	(414	12)	(415	2)	(416	40)	(421	6)
(422	12)	(426	9)	(427	6)	(434	11)	(438	27)
(441	11)	(444	7)	(448	9)	(452	1)	(453	5)
(455	10)	(459	33)	(460	21)	(463	10)	(467	30)
(470	2)	(471	40)	(472	3)	(473	7)	(480	32)
(484	19)	(485	6)	(489	32)	(490	22)	(491	23)
(493	15)	(494	42)	(498	29)	(505	3)	(513	21)
(514	32)	(517	28)	(520	27)	(522	10)	(525	1)
(529	31)	(534	6)	(541	22)	(542	8)	(554	5)
(557	3)	(558	13)	(559	5)	(561	11)	(572	3)
(573	9)	(577	29)	(579	12)	(582	4)	(583	21)
(587	4)	(588	5)	(592	14)	(593	6)	(595	12)
(598	3)	(599	12)						

NAME:13C\_1283.2\_1313EC11\_Urea (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:127002-11-1

RI:1283

RT:6.186

NUM PEAKS: 410

( 70	54)	( 71	41)	( 72	86)	( 73	263)	( 74	200)
( 75	57)	( 76	9)	( 77	9)	( 78	36)	( 79	62)
( 80	10)	( 82	5)	( 83	4)	( 84	5)	( 85	14)
( 86	27)	( 87	54)	( 90	9)	( 92	6)	( 93	9)
( 94	8)	( 95	6)	( 97	7)	( 98	4)	( 99	26)
(100	103)	(101	95)	(102	33)	(103	25)	(105	6)
(107	7)	(108	7)	(109	5)	(111	5)	(112	9)
(113	12)	(114	12)	(115	29)	(116	41)	(117	17)
(121	5)	(122	6)	(123	12)	(125	14)	(126	13)
(127	5)	(128	9)	(129	9)	(130	71)	(131	76)
(132	88)	(133	25)	(137	7)	(138	5)	(139	5)
(140	7)	(141	5)	(142	5)	(143	8)	(144	8)
(146	62)	(147	1000)	(148	210)	(149	90)	(150	14)
(151	5)	(152	7)	(153	7)	(154	6)	(155	6)
(156	7)	(157	8)	(158	11)	(159	7)	(160	10)
(163	9)	(164	8)	(167	6)	(168	7)	(169	4)
(170	6)	(171	38)	(172	101)	(173	33)	(174	45)
(177	8)	(178	8)	(179	5)	(180	5)	(182	5)
(183	3)	(184	5)	(185	7)	(186	5)	(187	8)
(188	6)	(189	98)	(190	259)	(191	51)	(192	27)
(193	7)	(194	6)	(195	5)	(196	6)	(197	4)
(198	7)	(200	4)	(203	3)	(204	12)	(205	17)
(206	10)	(207	8)	(208	5)	(209	4)	(212	5)
(213	6)	(214	5)	(215	5)	(216	5)	(217	6)
(218	5)	(220	5)	(222	10)	(223	5)	(224	5)
(225	5)	(226	8)	(227	4)	(229	6)	(230	8)
(231	7)	(232	5)	(233	5)	(234	5)	(235	6)
(236	7)	(238	4)	(239	8)	(240	7)	(242	3)
(243	5)	(244	6)	(245	5)	(247	3)	(248	5)
(249	4)	(250	2)	(251	5)	(252	6)	(254	4)
(256	3)	(257	6)	(258	5)	(259	5)	(260	4)
(261	3)	(263	5)	(264	5)	(265	6)	(266	4)
(267	6)	(268	7)	(269	8)	(270	7)	(271	10)
(272	6)	(273	6)	(275	16)	(276	8)	(277	8)
(278	8)	(279	8)	(280	7)	(281	6)	(283	5)
(284	5)	(287	8)	(288	8)	(289	11)	(290	7)
(292	4)	(293	10)	(294	6)	(295	5)	(296	4)
(297	6)	(298	4)	(300	4)	(301	3)	(302	4)
(303	6)	(304	3)	(306	3)	(307	2)	(308	4)
(309	5)	(310	4)	(312	6)	(314	6)	(315	5)
(316	7)	(317	7)	(318	5)	(319	6)	(320	5)
(322	3)	(323	6)	(326	7)	(327	5)	(328	8)
(329	6)	(330	6)	(331	3)	(332	6)	(333	7)
(334	5)	(335	4)	(336	5)	(337	5)	(339	5)
(340	5)	(341	2)	(342	5)	(343	7)	(344	4)
(345	4)	(346	5)	(347	9)	(348	6)	(349	4)
(351	6)	(352	6)	(353	5)	(354	7)	(355	8)
(357	6)	(358	7)	(359	8)	(360	11)	(361	9)
(362	8)	(363	5)	(364	13)	(365	6)	(366	6)
(367	8)	(368	5)	(369	7)	(371	9)	(373	5)
(374	3)	(375	7)	(376	7)	(377	6)	(378	8)
(379	13)	(380	5)	(381	5)	(383	9)	(389	11)
(391	5)	(392	5)	(393	6)	(394	4)	(395	7)
(397	5)	(398	5)	(400	6)	(401	5)	(402	6)
(403	5)	(404	5)	(405	6)	(406	4)	(407	3)
(408	5)	(409	4)	(410	6)	(411	9)	(412	5)
(415	6)	(416	5)	(417	6)	(419	6)	(420	4)



(421	6)	(422	4)	(423	3)	(424	3)	(426	4)
(427	6)	(430	4)	(431	3)	(432	5)	(433	6)
(434	5)	(435	6)	(437	5)	(438	3)	(440	6)
(441	5)	(442	4)	(444	4)	(445	5)	(446	5)
(447	5)	(448	7)	(449	4)	(450	6)	(451	5)
(454	5)	(455	4)	(457	4)	(458	6)	(459	5)
(460	6)	(461	5)	(462	6)	(463	9)	(464	5)
(466	3)	(467	5)	(468	3)	(469	3)	(470	8)
(471	8)	(472	8)	(473	7)	(475	2)	(476	6)
(477	7)	(479	6)	(480	5)	(482	7)	(484	7)
(486	5)	(487	17)	(489	7)	(490	5)	(491	6)
(492	5)	(493	5)	(495	3)	(498	8)	(499	7)
(500	6)	(501	4)	(502	5)	(503	6)	(504	5)
(505	6)	(506	6)	(507	7)	(508	4)	(510	5)
(511	3)	(512	2)	(513	6)	(514	5)	(515	6)
(516	5)	(517	5)	(518	6)	(519	8)	(522	6)
(523	5)	(524	5)	(525	6)	(528	3)	(529	5)
(530	5)	(531	4)	(532	6)	(533	6)	(534	7)
(536	3)	(537	6)	(539	4)	(540	7)	(541	7)
(542	4)	(544	6)	(545	6)	(546	3)	(547	5)
(548	7)	(551	3)	(552	5)	(553	3)	(554	4)
(555	7)	(556	4)	(561	5)	(562	3)	(563	6)
(564	4)	(566	6)	(567	5)	(568	4)	(569	4)
(572	5)	(574	2)	(575	5)	(577	3)	(579	3)
(582	2)	(588	3)	(589	2)	(590	3)	(591	3)

NAME:13C\_2223.0\_1313EC16\_Tryptophan (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:223001-11-1

RI:2223

RT:13.883

NUM PEAKS: 161

( 72	59)	( 73	320)	( 74	110)	( 75	153)	( 76	19)
( 80	12)	( 87	41)	( 88	38)	( 89	48)	( 95	15)
(101	36)	(102	56)	(110	28)	(116	8)	(120	9)
(124	8)	(130	8)	(136	10)	(137	23)	(138	38)
(139	22)	(141	18)	(143	10)	(151	7)	(153	12)
(157	7)	(162	12)	(167	7)	(170	4)	(173	7)
(174	5)	(175	11)	(177	8)	(179	15)	(195	6)
(196	7)	(197	8)	(200	4)	(203	14)	(204	11)
(209	27)	(210	108)	(211	1000)	(212	79)	(213	28)
(216	7)	(217	7)	(219	6)	(229	5)	(231	4)
(232	5)	(237	11)	(240	8)	(247	4)	(249	5)
(251	6)	(258	7)	(259	4)	(263	5)	(270	5)
(274	5)	(276	3)	(280	6)	(281	5)	(290	4)
(291	6)	(292	5)	(294	3)	(295	4)	(307	3)
(313	5)	(314	7)	(316	5)	(317	5)	(329	2)
(330	4)	(334	4)	(335	4)	(351	5)	(352	2)
(353	4)	(355	7)	(373	4)	(378	3)	(379	4)
(384	3)	(386	4)	(388	3)	(391	3)	(396	4)
(397	4)	(405	3)	(407	6)	(408	6)	(410	4)
(413	5)	(417	6)	(418	5)	(422	9)	(424	4)
(425	2)	(426	6)	(427	2)	(431	3)	(433	4)
(438	3)	(441	4)	(442	4)	(445	3)	(446	5)
(447	5)	(448	3)	(455	4)	(462	4)	(465	4)
(467	1)	(471	6)	(475	4)	(477	5)	(479	2)
(481	3)	(482	5)	(486	4)	(488	5)	(489	5)
(493	3)	(496	7)	(497	4)	(498	3)	(499	4)
(500	3)	(502	3)	(509	3)	(513	3)	(516	4)
(517	2)	(518	2)	(520	4)	(523	4)	(527	2)

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(532	4)	(536	4)	(537	2)	(538	4)	(541	4)
(542	3)	(543	6)	(546	3)	(547	3)	(550	2)
(552	4)	(555	3)	(558	2)	(564	3)	(566	3)
(567	4)	(571	2)	(573	2)	(574	2)	(591	2)
(595	2)								

NAME:13C\_2767.9\_1313EC16

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:277004-11-1

RI:2767

RT:16.765

NUM PEAKS: 93

( 70	41)	( 72	34)	( 73	1000)	( 74	107)	( 76	39)
( 78	24)	( 82	14)	( 83	31)	( 84	35)	( 91	22)
( 92	19)	( 93	18)	( 97	17)	( 98	22)	( 99	25)
(100	21)	(102	40)	(103	55)	(105	32)	(106	48)
(107	56)	(111	34)	(112	80)	(113	31)	(117	32)
(118	68)	(124	32)	(126	12)	(127	18)	(129	47)
(131	35)	(138	16)	(139	31)	(140	162)	(141	348)
(142	16)	(145	24)	(146	55)	(151	18)	(152	13)
(153	15)	(154	42)	(155	21)	(167	11)	(168	21)
(169	148)	(170	718)	(171	19)	(173	18)	(174	266)
(176	24)	(178	130)	(179	769)	(180	79)	(181	67)
(183	20)	(193	399)	(194	30)	(195	33)	(196	13)
(197	33)	(198	18)	(206	179)	(207	48)	(211	32)
(212	26)	(213	52)	(214	15)	(215	10)	(216	12)
(223	15)	(224	17)	(241	23)	(243	12)	(249	26)
(254	10)	(270	18)	(271	20)	(272	22)	(273	35)
(274	12)	(282	12)	(283	12)	(347	10)	(348	12)
(385	11)	(404	17)	(405	10)	(429	8)	(436	11)
(437	18)	(494	10)	(523	15)				

NAME:13C\_1915.4\_2119DC05\_Lysine (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:192003-11-1

RI:1915

RT:28.691

NUM PEAKS: 222

( 40	3)	( 41	58)	( 42	5)	( 43	19)	( 44	18)
( 45	84)	( 46	5)	( 47	6)	( 50	2)	( 51	8)
( 52	5)	( 53	14)	( 54	2)	( 55	59)	( 56	10)
( 57	104)	( 58	19)	( 59	126)	( 60	15)	( 61	8)
( 62	1)	( 63	4)	( 64	3)	( 65	13)	( 66	5)
( 67	20)	( 68	2)	( 69	8)	( 70	3)	( 72	25)
( 73	1000)	( 74	116)	( 75	82)	( 76	7)	( 77	23)
( 78	6)	( 79	20)	( 80	3)	( 81	9)	( 82	3)
( 83	6)	( 86	12)	( 87	139)	( 88	21)	( 89	85)
( 90	5)	( 91	34)	( 92	4)	( 93	8)	( 94	2)
( 95	10)	( 96	4)	( 97	5)	( 98	2)	(100	20)
(101	91)	(102	73)	(103	58)	(105	15)	(106	3)
(107	11)	(108	2)	(109	18)	(110	4)	(111	6)
(112	1)	(114	7)	(115	55)	(116	29)	(117	127)
(118	23)	(120	3)	(121	10)	(122	2)	(123	8)
(124	5)	(126	1)	(127	3)	(128	16)	(129	37)
(130	64)	(131	270)	(132	51)	(133	59)	(134	8)
(135	19)	(136	5)	(137	8)	(138	2)	(139	2)
(140	1)	(141	4)	(142	4)	(143	11)	(144	11)
(145	58)	(146	65)	(147	126)	(148	29)	(149	21)
(150	7)	(151	5)	(152	3)	(153	7)	(154	8)
(155	2)	(156	14)	(157	8)	(158	7)	(159	68)

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(160	59)	(161	691)	(162	55)	(163	36)	(164	5)
(165	5)	(166	1)	(167	1)	(170	1)	(171	3)
(172	11)	(173	24)	(175	666)	(176	117)	(177	85)
(178	13)	(179	6)	(180	1)	(185	2)	(186	3)
(187	8)	(188	6)	(189	58)	(190	23)	(191	16)
(192	26)	(193	5)	(194	3)	(199	1)	(200	2)
(201	7)	(202	5)	(203	66)	(204	22)	(205	98)
(206	21)	(213	1)	(215	2)	(217	53)	(218	39)
(219	18)	(220	66)	(221	17)	(222	8)	(223	1)
(228	1)	(229	1)	(230	3)	(231	3)	(232	21)
(233	66)	(234	124)	(235	50)	(236	15)	(237	2)
(238	1)	(243	1)	(244	1)	(245	3)	(246	5)
(247	4)	(249	4)	(250	1)	(251	1)	(257	1)
(260	1)	(261	16)	(262	5)	(263	2)	(264	4)
(265	2)	(271	1)	(276	3)	(277	3)	(278	8)
(279	7)	(280	2)	(291	1)	(292	1)	(299	9)
(300	2)	(301	1)	(305	1)	(306	1)	(307	2)
(308	2)	(309	1)	(317	3)	(318	1)	(319	1)
(320	1)	(321	6)	(322	174)	(323	39)	(324	21)
(325	4)	(326	1)	(333	1)	(334	1)	(335	17)
(336	7)	(337	3)	(396	3)	(397	1)	(425	4)
(426	1)	(427	1)	(439	1)	(440	19)	(441	7)
(442	4)	(443	1)						

NAME:13C\_1920.1\_2119DC05\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:192007-11-1

RI:1920

RT:28.753

NUM PEAKS: 81

( 43	35)	( 44	17)	( 45	80)	( 47	12)	( 58	64)
( 71	61)	( 72	24)	( 73	1000)	( 74	88)	( 75	149)
( 76	8)	( 84	12)	( 85	35)	( 86	15)	(113	7)
(118	24)	(131	28)	(132	22)	(133	36)	(140	3)
(147	445)	(148	62)	(149	62)	(160	17)	(169	6)
(174	17)	(203	35)	(204	5)	(206	14)	(221	34)
(223	5)	(229	3)	(231	6)	(247	3)	(248	153)
(249	33)	(250	18)	(259	2)	(263	3)	(264	12)
(277	20)	(278	7)	(279	5)	(290	2)	(291	4)
(292	8)	(293	303)	(294	56)	(295	29)	(296	4)
(297	2)	(305	3)	(306	12)	(307	13)	(308	11)
(309	4)	(311	4)	(319	32)	(320	12)	(321	8)
(324	6)	(338	12)	(339	3)	(352	12)	(353	6)
(354	3)	(366	4)	(367	68)	(368	20)	(369	7)
(370	3)	(378	2)	(383	32)	(384	8)	(385	4)
(396	22)	(397	5)	(468	3)	(486	27)	(487	8)
(488	5)								

NAME:13C\_1858.1\_2119DC05\_Lysine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1858 |RI:1858

CASNO:186002-11-1

RI:1858

RT:27.441

SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp

NUM PEAKS: 119

( 44	26)	( 45	125)	( 46	12)	( 47	13)	( 48	1)
( 50	1)	( 51	1)	( 52	2)	( 58	15)	( 59	185)
( 60	20)	( 61	11)	( 62	1)	( 70	3)	( 72	19)
( 73	789)	( 74	139)	( 76	11)	( 78	1)	( 85	4)
( 86	13)	( 87	199)	( 88	34)	( 89	233)	( 90	7)

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( 91	2)	( 92	1)	(100	27)	(101	85)	(102	28)
(103	33)	(104	19)	(106	1)	(110	1)	(113	4)
(114	6)	(115	21)	(116	16)	(118	15)	(119	8)
(120	2)	(128	2)	(130	47)	(131	76)	(133	25)
(134	5)	(135	2)	(142	1)	(144	4)	(146	49)
(147	72)	(148	26)	(149	9)	(150	2)	(156	3)
(157	1)	(158	2)	(159	13)	(160	18)	(161	210)
(162	25)	(163	11)	(164	2)	(172	6)	(173	28)
(174	66)	(175	1000)	(176	170)	(177	80)	(178	9)
(179	2)	(188	3)	(189	10)	(190	12)	(192	9)
(193	2)	(200	3)	(202	1)	(203	14)	(204	5)
(205	13)	(206	176)	(207	20)	(208	8)	(217	1)
(218	2)	(219	2)	(220	9)	(230	1)	(232	1)
(233	2)	(234	4)	(235	30)	(236	8)	(237	3)
(238	1)	(245	6)	(246	2)	(247	2)	(248	3)
(249	2)	(250	1)	(261	2)	(262	1)	(263	6)
(264	47)	(265	8)	(266	4)	(278	1)	(294	1)
(295	6)	(296	1)	(297	1)	(336	1)	(353	2)
(367	1)	(368	20)	(369	5)	(370	2)		

NAME:13C\_1490.2\_2119DC05\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:149003-11-1

RI:1490

RT:20.226

NUM PEAKS: 155

( 42	41)	( 43	38)	( 44	220)	( 45	159)	( 46	109)
( 47	38)	( 51	16)	( 52	19)	( 56	10)	( 57	23)
( 59	236)	( 60	49)	( 61	112)	( 62	15)	( 64	3)
( 65	3)	( 66	11)	( 69	8)	( 70	14)	( 71	8)
( 72	76)	( 73	1000)	( 74	208)	( 75	701)	( 76	80)
( 77	52)	( 79	27)	( 80	4)	( 85	8)	( 86	20)
( 87	35)	( 88	54)	( 89	68)	( 90	253)	( 91	31)
( 92	26)	( 94	9)	( 99	4)	(100	14)	(101	70)
(102	28)	(104	27)	(107	5)	(113	5)	(115	13)
(116	12)	(117	25)	(118	91)	(119	64)	(122	6)
(126	7)	(129	12)	(130	16)	(132	12)	(134	36)
(135	20)	(145	14)	(146	75)	(147	952)	(148	301)
(149	96)	(150	15)	(155	3)	(158	7)	(160	4)
(161	19)	(162	116)	(163	119)	(164	154)	(165	40)
(166	17)	(174	3)	(179	14)	(180	7)	(181	5)
(183	2)	(192	191)	(193	50)	(194	21)	(195	3)
(196	5)	(200	3)	(202	3)	(204	5)	(208	40)
(209	146)	(210	26)	(211	17)	(216	2)	(220	19)
(222	5)	(224	6)	(235	21)	(237	41)	(239	3)
(241	2)	(242	3)	(252	14)	(253	67)	(254	13)
(255	8)	(256	3)	(258	2)	(260	3)	(264	3)
(271	3)	(279	3)	(280	10)	(281	135)	(282	26)
(283	16)	(284	2)	(285	2)	(287	3)	(295	3)
(297	7)	(298	30)	(299	4)	(300	9)	(303	2)
(322	4)	(327	26)	(328	7)	(329	4)	(342	2)
(345	3)	(346	2)	(349	3)	(350	2)	(354	2)
(358	3)	(407	4)	(412	3)	(413	3)	(433	2)
(445	3)	(447	5)	(449	4)	(454	3)	(459	2)
(463	2)	(474	2)	(478	3)	(491	2)	(495	2)
(503	3)	(512	2)	(533	2)	(545	2)	(553	3)
(556	2)	(562	2)	(568	3)	(570	3)	(597	3)

NAME:13C\_2816.0\_2119DC05\_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:282003-11-1

RI:2816

RT:41.157

NUM PEAKS: 36

( 46	17)	( 73	1000)	( 74	77)	( 75	76)	(104	215)
(132	227)	(133	65)	(147	285)	(148	36)	(160	54)
(161	50)	(174	153)	(178	14)	(186	13)	(188	11)
(192	358)	(193	75)	(194	44)	(206	128)	(208	24)
(218	14)	(220	305)	(221	69)	(222	23)	(233	22)
(236	22)	(248	74)	(263	13)	(277	83)	(308	25)
(323	33)	(336	46)	(367	386)	(368	92)	(369	49)
(370	12)								

NAME:12C\_1731.5\_1313EC36\_Ribitol (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:173001-10-1

RI:1731

RT:10.548

NUM PEAKS: 84

( 70	4)	( 71	5)	( 72	21)	( 73	1000)	( 74	87)
( 75	73)	( 76	3)	( 77	3)	( 81	8)	( 83	5)
( 85	4)	( 87	8)	( 88	6)	( 89	28)	( 90	3)
( 99	5)	(101	28)	(102	5)	(103	225)	(104	22)
(105	10)	(111	3)	(113	6)	(115	6)	(116	10)
(117	95)	(118	9)	(119	9)	(129	129)	(130	16)
(131	33)	(132	5)	(133	70)	(134	10)	(135	6)
(142	3)	(143	10)	(145	4)	(147	309)	(148	49)
(149	31)	(150	3)	(155	6)	(157	24)	(158	3)
(159	3)	(161	3)	(163	5)	(170	3)	(171	3)
(175	6)	(177	3)	(189	55)	(190	12)	(191	24)
(192	4)	(203	14)	(204	48)	(205	106)	(206	22)
(207	12)	(217	242)	(218	65)	(219	25)	(220	4)
(221	9)	(229	7)	(231	3)	(243	15)	(244	4)
(277	10)	(278	4)	(291	4)	(306	4)	(307	30)
(308	9)	(309	4)	(317	5)	(318	5)	(319	50)
(320	16)	(321	7)	(332	10)	(333	4)		

NAME:12C\_1316.0\_1313EC36\_Isoleucine (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:132002-10-1

RI:1316

RT:6.560

NUM PEAKS: 44

( 70	19)	( 71	7)	( 72	26)	( 73	895)	( 82	4)
( 84	12)	( 85	11)	( 86	48)	( 89	4)	( 90	8)
( 96	6)	( 97	4)	( 98	12)	( 99	7)	(100	126)
(102	39)	(103	21)	(105	3)	(112	5)	(113	4)
(126	3)	(128	27)	(129	20)	(133	34)	(134	8)
(145	3)	(147	137)	(149	16)	(156	7)	(158	1000)
(159	149)	(160	48)	(161	5)	(163	5)	(170	15)
(171	3)	(174	3)	(203	9)	(217	3)	(218	142)
(232	38)	(233	12)	(260	7)	(261	2)		

NAME:12C\_1436.0\_1313EC36\_[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:143003-10-1

RI:1436

RT:7.989

NUM PEAKS: 26

136

( 73 1000) ( 74 109) ( 82 77) ( 85 30) ( 86 334)  
( 87 39) ( 89 58) ( 99 28) (100 186) (102 163)  
(113 38) (114 26) (117 29) (126 26) (128 32)  
(130 75) (154 393) (155 90) (156 130) (158 17)  
(172 55) (174 538) (175 96) (176 35) (186 32)  
(227 34)

NAME:12C\_1459.3\_1313EC36\_Homoserine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:146001-10-1

RI:1459

RT:8.266

NUM PEAKS: 72

( 70 8) ( 71 13) ( 72 26) ( 73 1000) ( 74 95)  
( 75 119) ( 76 11) ( 77 5) ( 82 6) ( 83 3)  
( 84 15) ( 85 5) ( 86 10) ( 87 9) ( 88 4)  
( 98 11) (100 107) (101 22) (102 45) (103 235)  
(104 23) (105 12) (112 8) (113 4) (114 14)  
(115 8) (116 7) (117 15) (119 7) (127 4)  
(128 397) (129 58) (130 63) (131 43) (132 25)  
(133 62) (134 10) (135 5) (137 3) (143 4)  
(144 6) (145 3) (146 19) (156 7) (158 9)  
(160 4) (163 4) (172 6) (174 10) (175 4)  
(176 4) (178 3) (186 4) (188 8) (189 4)  
(191 3) (202 32) (203 8) (204 6) (214 4)  
(216 11) (217 6) (218 503) (219 112) (220 42)  
(221 8) (230 17) (231 4) (232 8) (292 17)  
(293 6) (320 6)

NAME:12C\_1495.6\_1313EC36\_[815; Ethyl-3(2H)-thiophenone]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:150003-10-1

RI:1496

RT:8.698

NUM PEAKS: 56

( 72 18) ( 73 546) ( 74 61) ( 75 165) ( 76 13)  
( 77 10) ( 82 5) ( 84 10) ( 86 11) ( 87 6)  
( 88 3) ( 96 3) ( 98 18) (100 67) (101 12)  
(102 9) (103 16) (104 3) (105 3) (112 9)  
(114 16) (115 12) (116 8) (117 41) (118 5)  
(119 5) (126 5) (128 1000) (129 133) (130 82)  
(131 18) (132 10) (133 23) (134 4) (144 5)  
(146 3) (148 11) (149 13) (156 7) (158 13)  
(172 4) (173 3) (174 5) (188 94) (189 13)  
(190 4) (200 3) (202 60) (203 12) (204 5)  
(216 3) (218 10) (219 3) (230 12) (290 4)  
(305 3)

NAME:12C\_1514.1\_1313EC36\_[729; N,N-Dimethyllysine methyl ester]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:151003-10-1

RI:1514

RT:8.860

NUM PEAKS: 29

( 72 40) ( 73 1000) ( 74 101) ( 75 258) ( 82 16)  
( 84 893) ( 87 12) ( 89 205) ( 98 119) (100 81)  
(105 28) (114 32) (116 18) (128 67) (131 30)  
(133 46) (140 41) (147 188) (148 29) (156 104)  
(157 14) (158 35) (172 23) (188 844) (189 112)  
(190 28) (200 16) (230 29) (274 20)

NAME:12C\_1538.2\_1313EC36\_[596; N-Acetylglutamic acid (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:154002-10-1

RI:1538

RT:9.048

NUM PEAKS: 61

( 72	46)	( 73	454)	( 74	75)	( 75	623)	( 76	52)
( 77	33)	( 83	17)	( 84	1000)	( 86	12)	( 87	18)
( 88	13)	( 89	9)	( 90	3)	( 91	6)	(101	19)
(102	10)	(103	18)	(104	3)	(112	10)	(114	7)
(115	7)	(116	31)	(118	4)	(129	25)	(130	34)
(131	24)	(132	5)	(133	22)	(134	3)	(140	40)
(141	6)	(142	9)	(143	3)	(144	12)	(145	14)
(146	19)	(147	62)	(148	10)	(149	13)	(156	57)
(157	15)	(158	202)	(159	30)	(160	13)	(173	21)
(174	400)	(175	52)	(176	16)	(186	68)	(187	8)
(201	17)	(202	3)	(230	35)	(231	8)	(232	3)
(248	14)	(249	3)	(258	4)	(276	33)	(277	7)
(278	3)								

NAME:12C\_1623.5\_1313EC36\_[882; Ornithine (3TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:162001-10-1

RI:1624

RT:9.710

NUM PEAKS: 109

( 70	553)	( 71	37)	( 72	35)	( 73	1000)	( 74	231)
( 75	128)	( 76	13)	( 77	5)	( 80	4)	( 82	5)
( 83	4)	( 84	13)	( 85	10)	( 86	21)	( 87	12)
( 88	15)	( 89	26)	( 90	7)	( 96	7)	( 97	14)
( 98	20)	( 99	9)	(100	96)	(101	19)	(102	115)
(103	26)	(104	11)	(105	3)	(108	3)	(110	5)
(112	6)	(113	6)	(114	24)	(115	75)	(116	19)
(117	41)	(118	7)	(119	5)	(126	9)	(127	4)
(128	65)	(129	30)	(130	32)	(131	25)	(132	29)
(133	34)	(134	7)	(135	3)	(140	9)	(141	10)
(142	661)	(143	104)	(144	92)	(145	12)	(146	22)
(147	108)	(148	34)	(149	14)	(150	3)	(152	3)
(153	16)	(154	13)	(155	4)	(157	7)	(158	7)
(159	5)	(160	4)	(162	60)	(163	11)	(164	5)
(168	3)	(169	14)	(170	8)	(171	5)	(172	9)
(173	3)	(174	7)	(186	4)	(187	4)	(188	9)
(189	5)	(190	3)	(191	4)	(200	7)	(203	3)
(204	43)	(205	9)	(206	4)	(214	4)	(215	5)
(216	33)	(217	16)	(218	22)	(219	9)	(220	3)
(227	4)	(231	7)	(232	8)	(233	3)	(241	4)
(243	31)	(244	27)	(245	8)	(258	7)	(259	12)
(260	3)	(348	27)	(349	9)	(350	4)		

NAME:12C\_1640.8\_1313EC36\_Phenylalanine (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:164001-10-1

RI:1641

RT:9.844

NUM PEAKS: 63

( 71	5)	( 72	21)	( 73	1000)	( 74	94)	( 75	110)
( 76	8)	( 77	15)	( 78	5)	( 86	18)	( 87	6)
( 89	12)	( 90	6)	( 91	174)	( 92	26)	( 93	5)
(100	189)	(101	26)	(103	21)	(104	5)	(105	7)

138

(115	8)	(116	3)	(117	15)	(118	10)	(119	10)
(120	12)	(121	9)	(130	41)	(131	26)	(132	31)
(133	34)	(134	7)	(135	9)	(145	5)	(146	12)
(147	159)	(148	27)	(149	15)	(159	5)	(160	18)
(161	5)	(162	7)	(163	10)	(174	5)	(176	10)
(177	12)	(178	3)	(190	3)	(191	7)	(192	282)
(193	53)	(194	13)	(203	7)	(204	11)	(205	3)
(217	4)	(218	397)	(219	77)	(220	33)	(266	24)
(267	13)	(268	4)	(294	6)				

NAME:12C\_1673.2\_1313EC36\_[NA]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:167003-10-1

RI:1673

RT:10.095

NUM PEAKS: 66

( 70	28)	( 73	1000)	( 74	100)	( 82	142)	( 84	9)
( 98	500)	( 99	37)	(101	8)	(110	18)	(114	17)
(116	11)	(130	10)	(140	5)	(154	5)	(156	50)
(157	11)	(170	36)	(176	4)	(184	14)	(186	4)
(198	5)	(199	4)	(200	13)	(216	9)	(221	5)
(230	4)	(231	10)	(232	9)	(244	14)	(249	4)
(252	4)	(267	5)	(279	4)	(287	21)	(288	458)
(289	117)	(290	45)	(291	8)	(293	5)	(318	6)
(319	6)	(322	4)	(324	4)	(336	7)	(337	4)
(344	4)	(346	10)	(347	6)	(391	5)	(398	4)
(408	5)	(409	4)	(410	5)	(423	5)	(431	5)
(439	4)	(447	4)	(478	4)	(481	6)	(490	5)
(515	5)	(532	4)	(548	4)	(558	4)	(567	3)
(570	3)								

NAME:12C\_1708.2\_1313EC36\_[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:171003-10-1

RI:1708

RT:10.367

NUM PEAKS: 91

( 70	22)	( 71	9)	( 72	25)	( 73	1000)	( 74	81)
( 75	114)	( 79	9)	( 81	14)	( 86	12)	( 87	8)
( 89	87)	(100	46)	(105	5)	(112	7)	(114	16)
(116	19)	(117	15)	(127	24)	(128	52)	(129	21)
(132	16)	(133	28)	(134	6)	(135	3)	(142	28)
(143	8)	(144	24)	(145	32)	(146	9)	(147	91)
(148	13)	(149	6)	(155	61)	(158	11)	(159	5)
(161	10)	(171	62)	(172	19)	(174	22)	(175	4)
(176	5)	(182	5)	(183	5)	(185	9)	(187	6)
(188	11)	(202	8)	(211	8)	(218	16)	(219	17)
(228	6)	(229	9)	(232	13)	(242	3)	(243	5)
(244	24)	(245	12)	(246	4)	(272	31)	(275	102)
(276	28)	(277	12)	(287	5)	(288	6)	(296	9)
(297	6)	(298	7)	(337	4)	(338	4)	(348	6)
(350	6)	(358	3)	(399	4)	(411	4)	(415	5)
(421	4)	(422	4)	(431	4)	(458	6)	(459	4)
(462	4)	(470	3)	(479	4)	(483	5)	(513	5)
(515	5)	(543	5)	(548	7)	(557	5)	(558	4)
(588	4)								

NAME:12C\_1720.9\_1313EC36\_[NA]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer



CASNO:172005-10-1

RI:1721

RT:10.465

NUM PEAKS: 56

( 70	46)	( 72	90)	( 73	789)	( 74	188)	( 75	1000)
( 76	84)	( 77	54)	( 81	16)	( 83	199)	( 86	17)
( 87	41)	( 90	180)	( 94	9)	(112	17)	(113	31)
(115	83)	(116	152)	(119	8)	(126	11)	(131	167)
(132	24)	(139	70)	(140	53)	(141	14)	(142	24)
(145	42)	(146	18)	(149	13)	(155	266)	(156	429)
(157	135)	(158	132)	(159	23)	(160	40)	(162	9)
(171	8)	(172	31)	(173	617)	(174	88)	(175	39)
(185	10)	(186	22)	(187	13)	(199	8)	(202	14)
(223	8)	(229	74)	(236	10)	(254	8)	(255	13)
(261	10)	(262	8)	(268	8)	(275	23)	(276	13)
(285	7)								

NAME:12C\_1747.3\_1313EC36\_[612; 4-Aminobutyric acid (2TBS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:175003-10-1

RI:1747

RT:10.670

NUM PEAKS: 19

( 73	1000)	( 74	93)	( 75	182)	( 78	34)	( 84	207)
(100	39)	(112	314)	(115	34)	(129	51)	(131	27)
(133	53)	(147	369)	(148	60)	(149	43)	(156	48)
(184	29)	(194	48)	(274	267)	(275	59)		

NAME:12C\_1784.4\_1313EC36\_Glutamine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:178001-10-1

RI:1785

RT:10.958

NUM PEAKS: 107

( 70	19)	( 71	11)	( 72	44)	( 73	1000)	( 74	138)
( 75	301)	( 76	23)	( 77	12)	( 81	5)	( 82	6)
( 83	35)	( 84	26)	( 85	12)	( 86	14)	( 87	8)
( 88	4)	( 89	6)	( 90	5)	( 94	3)	( 96	3)
( 97	3)	( 98	11)	( 99	7)	(100	63)	(101	14)
(102	11)	(105	3)	(110	3)	(112	17)	(113	11)
(114	44)	(115	41)	(116	37)	(117	16)	(118	4)
(119	5)	(126	13)	(127	4)	(128	77)	(129	23)
(130	26)	(131	72)	(132	26)	(133	52)	(134	9)
(135	5)	(139	50)	(140	22)	(141	7)	(142	22)
(143	5)	(144	8)	(145	36)	(146	10)	(147	163)
(148	32)	(149	34)	(150	5)	(151	3)	(153	3)
(154	4)	(155	244)	(156	775)	(157	121)	(158	37)
(159	5)	(160	3)	(167	3)	(172	8)	(173	9)
(174	5)	(183	3)	(188	15)	(189	5)	(190	3)
(200	3)	(202	3)	(203	64)	(204	16)	(205	6)
(211	3)	(213	3)	(214	3)	(216	8)	(218	17)
(219	5)	(221	4)	(227	7)	(228	5)	(229	27)
(230	16)	(231	5)	(232	10)	(244	6)	(245	97)
(246	22)	(247	8)	(257	6)	(258	3)	(272	5)
(273	7)	(274	3)	(301	7)	(302	3)	(347	16)
(348	5)	(362	6)						

NAME:12C\_1843.5\_1313EC36\_[919; D-Xylopyranose (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:184004-10-1

140

RI:1844

RT:11.416

NUM PEAKS: 29

( 72	19)	( 73	1000)	( 74	85)	( 75	114)	( 76	7)
( 89	12)	(101	32)	(103	63)	(117	53)	(129	54)
(131	28)	(133	58)	(134	8)	(143	20)	(147	218)
(148	33)	(149	27)	(189	35)	(191	248)	(192	42)
(193	18)	(203	9)	(204	332)	(205	69)	(206	24)
(217	125)	(218	28)	(219	13)	(305	7)		

NAME:12C\_1858.1\_1313EC36\_Lysine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1858 |RI:1858 |RI:1858

CASNO:186002-10-1

RI:1858

RT:11.530

SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp

NUM PEAKS: 99

( 70	22)	( 71	11)	( 72	24)	( 73	1000)	( 74	161)
( 75	194)	( 76	18)	( 77	8)	( 80	6)	( 81	3)
( 82	59)	( 83	11)	( 84	200)	( 85	25)	( 86	214)
( 87	28)	( 88	41)	( 89	6)	( 90	3)	( 94	14)
( 95	3)	( 97	6)	( 98	12)	( 99	11)	(100	120)
(101	22)	(102	40)	(103	19)	(104	4)	(110	7)
(111	3)	(112	24)	(113	10)	(114	39)	(115	17)
(116	20)	(117	24)	(118	6)	(119	4)	(126	7)
(127	3)	(128	56)	(129	15)	(130	71)	(131	34)
(132	21)	(133	21)	(134	4)	(140	10)	(141	3)
(142	27)	(143	7)	(144	15)	(145	4)	(146	35)
(147	67)	(148	20)	(149	8)	(154	7)	(155	5)
(156	177)	(157	28)	(158	20)	(159	4)	(160	7)
(161	3)	(162	4)	(166	4)	(167	7)	(168	39)
(169	6)	(170	5)	(172	19)	(173	5)	(174	916)
(175	169)	(176	74)	(177	8)	(183	4)	(184	8)
(186	15)	(187	4)	(188	4)	(199	3)	(200	191)
(201	35)	(202	12)	(216	7)	(230	23)	(231	6)
(232	3)	(257	4)	(258	46)	(259	10)	(260	4)
(289	6)	(347	3)	(362	16)	(363	6)		

NAME:12C\_1888.7\_1313EC36\_[772; D-Glucose (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:189005-10-1

RI:1889

RT:11.768

NUM PEAKS: 6

(169	14)	(191	549)	(192	88)	(193	40)	(204	1000)
(398	3)								

NAME:12C\_1892.7\_1313EC36\_Tyrosine (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:189006-10-1

RI:1893

RT:11.798

NUM PEAKS: 47

( 75	399)	( 76	36)	( 77	44)	( 78	21)	( 79	15)
( 80	5)	( 82	63)	( 87	36)	( 90	52)	( 91	83)
( 92	10)	( 93	6)	( 95	8)	(107	14)	(109	5)
(118	34)	(119	58)	(120	7)	(121	8)	(123	3)
(135	43)	(136	5)	(137	5)	(146	71)	(150	8)
(151	20)	(163	41)	(164	19)	(165	34)	(166	8)
(175	12)	(176	15)	(177	16)	(178	16)	(179	1000)

141

(180 231) (181 57) (208 104) (209 21) (219 75)  
 (220 11) (265 5) (282 3) (293 6) (310 29)  
 (311 7) (312 3)

NAME:12C\_1973.7\_1313EC36\_[945; beta-D-Glucopyranose (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:197002-10-1

RI:1974

RT:12.324

NUM PEAKS: 66

( 73 1000) ( 74 83) ( 75 95) ( 76 5) ( 77 5)  
 ( 81 7) ( 83 3) ( 87 7) ( 88 4) ( 89 14)  
 (101 30) (102 5) (103 64) (104 5) (105 4)  
 (111 4) (113 3) (115 6) (116 14) (117 37)  
 (118 4) (119 6) (129 64) (130 8) (131 28)  
 (132 4) (133 56) (134 7) (135 5) (143 16)  
 (145 5) (147 223) (148 35) (155 4) (157 8)  
 (159 3) (161 3) (163 4) (169 9) (175 4)  
 (177 3) (189 38) (190 11) (191 266) (192 47)  
 (193 20) (203 12) (204 430) (205 84) (206 36)  
 (207 8) (217 83) (218 23) (219 9) (221 7)  
 (230 3) (231 9) (232 3) (233 3) (243 7)  
 (291 6) (305 6) (317 3) (319 3) (345 3)  
 (435 3)

NAME:12C\_1924.5\_1313EC16\_Histidine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:192006-10-1

RI:1925

RT:12.015

NUM PEAKS: 83

( 70 10) ( 71 5) ( 72 23) ( 73 1000) ( 74 88)  
 ( 75 87) ( 76 5) ( 81 43) ( 82 43) ( 83 17)  
 ( 84 18) ( 90 7) ( 96 6) ( 97 4) ( 98 8)  
 (104 34) (110 8) (111 6) (118 3) (119 25)  
 (120 3) (125 4) (126 10) (132 35) (133 21)  
 (134 4) (135 4) (137 3) (139 8) (147 95)  
 (148 15) (149 8) (150 6) (151 3) (153 47)  
 (154 1000) (155 214) (161 12) (165 3) (166 22)  
 (167 8) (180 3) (181 3) (182 14) (183 5)  
 (184 3) (191 9) (192 9) (193 3) (203 4)  
 (206 11) (207 30) (208 7) (209 3) (211 3)  
 (218 40) (219 8) (220 35) (222 3) (225 3)  
 (226 14) (227 4) (233 3) (235 4) (238 36)  
 (239 11) (240 4) (253 5) (254 171) (255 41)  
 (256 16) (257 10) (266 8) (310 4) (322 3)  
 (323 25) (324 7) (325 3) (328 5) (336 4)  
 (356 13) (357 5) (371 5)

NAME:12C\_2091.2\_1313EC11\_myoinositol (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:209002-10-1

RI:2091

RT:13.074

NUM PEAKS: 112

( 72 16) ( 73 1000) ( 74 86) ( 75 67) ( 76 3)  
 ( 81 9) ( 83 3) ( 85 3) ( 87 6) ( 97 3)  
 ( 99 6) (100 3) (103 57) (108 3) (111 8)  
 (113 6) (115 7) (116 7) (117 8) (125 3)  
 (127 4) (129 76) (130 11) (131 32) (133 74)

142

(134	11)	(135	6)	(141	4)	(142	3)	(143	23)
(144	6)	(147	319)	(148	50)	(149	20)	(154	3)
(155	4)	(156	4)	(157	7)	(159	4)	(167	3)
(169	4)	(175	13)	(177	7)	(189	15)	(190	13)
(191	103)	(192	24)	(193	10)	(195	3)	(201	4)
(203	7)	(204	43)	(205	15)	(215	4)	(216	5)
(217	168)	(218	35)	(219	17)	(230	7)	(231	5)
(242	3)	(243	7)	(244	3)	(245	3)	(254	3)
(260	3)	(265	27)	(266	9)	(267	5)	(291	15)
(292	6)	(293	6)	(304	11)	(305	98)	(306	32)
(307	18)	(308	6)	(317	8)	(318	55)	(319	25)
(320	11)	(321	4)	(331	3)	(343	3)	(344	3)
(345	3)	(353	3)	(365	3)	(367	7)	(368	5)
(369	3)	(379	3)	(391	3)	(392	3)	(393	5)
(394	3)	(398	3)	(403	3)	(408	3)	(417	3)
(421	3)	(430	3)	(431	3)	(432	10)	(433	8)
(434	6)	(435	3)	(444	3)	(454	3)	(506	3)
(507	5)	(508	3)						

NAME:12C\_1293.1\_1313EC75\_Glycerol (3TMS)  
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
 CASNO:129003-10-1

RI:1293

RT:6.323

NUM PEAKS: 58

( 70	4)	( 71	8)	( 72	25)	( 73	1000)	( 74	91)
( 75	90)	( 76	5)	( 85	9)	( 87	13)	( 88	13)
( 89	47)	( 90	5)	( 99	6)	(101	72)	(102	11)
(103	321)	(104	33)	(105	21)	(113	7)	(116	27)
(117	321)	(118	34)	(119	33)	(120	3)	(129	66)
(130	10)	(131	58)	(132	10)	(133	231)	(134	34)
(145	3)	(147	583)	(148	92)	(149	64)	(150	8)
(159	5)	(161	3)	(163	12)	(174	4)	(175	56)
(176	11)	(177	33)	(178	7)	(189	10)	(190	3)
(191	36)	(192	7)	(203	29)	(204	43)	(205	268)
(206	56)	(207	29)	(217	17)	(218	113)	(219	25)
(220	11)	(221	5)	(293	10)				

NAME:12C\_1317.6\_1313EC75\_Threonine (2TMS)  
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
 CASNO:132001-10-1

RI:1318

RT:6.611

NUM PEAKS: 51

( 71	11)	( 72	29)	( 73	1000)	( 74	129)	( 75	300)
( 76	25)	( 77	17)	( 81	5)	( 85	8)	( 86	8)
( 87	49)	( 88	10)	( 89	7)	( 91	3)	( 98	9)
(100	8)	(101	31)	(102	18)	(103	12)	(104	6)
(105	5)	(112	3)	(114	19)	(115	25)	(116	18)
(117	273)	(118	31)	(119	15)	(128	3)	(129	6)
(130	206)	(131	83)	(132	59)	(133	36)	(134	8)
(135	4)	(145	3)	(146	73)	(147	172)	(148	35)
(149	15)	(150	3)	(176	3)	(177	3)	(181	4)
(203	3)	(204	8)	(219	76)	(220	20)	(221	8)
(248	8)								

NAME:12C\_1318.4\_1313EC75\_Proline (2TMS)  
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
 CASNO:132003-10-1

RI:1318

143

RT:6.620

NUM PEAKS: 32

( 70	47)	( 71	10)	( 72	46)	( 73	608)	( 80	5)
( 83	3)	( 84	13)	( 85	7)	( 86	6)	( 96	3)
( 97	3)	( 98	7)	( 99	12)	(100	12)	(103	9)
(113	7)	(124	4)	(126	4)	(127	5)	(128	3)
(140	12)	(141	8)	(142	1000)	(143	137)	(144	39)
(145	3)	(147	80)	(170	10)	(175	5)	(216	44)
(217	9)	(244	5)						

NAME:12C\_1338.0\_1313EC75\_Succinic acid (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:134001-10-1

RI:1338

RT:6.850

NUM PEAKS: 32

( 72	29)	( 73	547)	( 75	415)	( 79	4)	( 86	13)
( 87	9)	( 89	10)	(101	9)	(102	4)	(113	6)
(115	12)	(116	18)	(117	14)	(129	95)	(130	4)
(131	23)	(133	46)	(143	5)	(145	5)	(147	1000)
(148	154)	(157	4)	(163	3)	(172	44)	(173	22)
(174	4)	(175	14)	(218	6)	(247	79)	(248	16)
(249	7)	(262	3)						

NAME:12C\_1378.1\_1313EC75\_Alanine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:138002-10-1

RI:1378

RT:7.321

NUM PEAKS: 54

( 70	24)	( 71	10)	( 72	28)	( 73	1000)	( 74	79)
( 84	3)	( 85	7)	( 86	12)	( 87	8)	( 98	3)
( 99	5)	(100	616)	(101	68)	(102	26)	(113	8)
(114	158)	(115	32)	(116	26)	(117	26)	(118	4)
(119	11)	(131	46)	(132	9)	(133	154)	(134	21)
(135	11)	(142	3)	(147	220)	(148	33)	(149	16)
(158	14)	(159	3)	(160	5)	(161	3)	(172	24)
(173	3)	(174	14)	(175	11)	(187	3)	(188	726)
(189	138)	(190	57)	(191	18)	(192	3)	(200	3)
(202	15)	(203	3)	(246	4)	(261	3)	(262	97)
(263	29)	(264	13)	(290	18)	(291	6)		

NAME:12C\_1381.0\_1313EC75\_Serine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:138001-10-1

RI:1381

RT:7.354

NUM PEAKS: 31

( 72	31)	( 73	1000)	( 74	96)	( 86	18)	( 88	19)
(102	16)	(116	71)	(118	8)	(119	8)	(135	6)
(147	138)	(148	26)	(149	19)	(160	5)	(163	7)
(174	15)	(203	11)	(204	348)	(205	68)	(206	27)
(207	4)	(216	13)	(217	6)	(218	178)	(219	36)
(220	16)	(221	5)	(278	18)	(279	7)	(306	9)
(307	4)								

NAME:12C\_1410.5\_1313EC75\_[700; 2-methyl-1,2-propanediol (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:141003-10-1

RI:1411

144

RT:7.700

NUM PEAKS: 33

( 73 1000)	(102 98)	(104 4)	(115 46)	(119 8)
(131 688)	(132 83)	(133 109)	(134 13)	(135 8)
(143 36)	(144 7)	(145 8)	(147 202)	(149 44)
(150 5)	(161 4)	(189 3)	(191 14)	(203 6)
(204 7)	(207 4)	(217 6)	(220 5)	(221 24)
(222 6)	(223 3)	(277 10)	(291 7)	(292 89)
(293 26)	(294 12)	(335 4)		

NAME:12C\_1419.8\_1313EC75\_Alanine {BP} (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:142001-10-1

RI:1420

RT:7.810

NUM PEAKS: 38

( 70 150)	( 72 50)	( 73 1000)	( 74 101)	( 75 344)
( 76 22)	( 86 38)	( 94 11)	(100 148)	(101 24)
(102 20)	(115 12)	(116 491)	(117 82)	(118 21)
(119 6)	(131 14)	(133 51)	(144 43)	(145 12)
(147 332)	(148 50)	(149 38)	(160 455)	(161 52)
(162 16)	(175 7)	(187 5)	(190 128)	(191 22)
(192 9)	(218 9)	(233 11)	(234 19)	(255 8)
(262 74)	(263 14)	(264 5)		

NAME:12C\_1464.2\_1313EC75\_[725; 2-Ketooctanoic acid (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:146003-10-1

RI:1464

RT:8.330

NUM PEAKS: 82

( 70 6)	( 71 8)	( 72 26)	( 73 674)	( 74 64)
( 75 249)	( 76 17)	( 77 24)	( 79 8)	( 80 3)
( 81 39)	( 82 4)	( 83 38)	( 84 7)	( 85 12)
( 86 3)	( 87 8)	( 89 4)	( 93 4)	( 94 12)
( 95 51)	( 96 61)	( 97 16)	( 98 7)	( 99 13)
(100 6)	(101 5)	(102 3)	(103 8)	(105 4)
(109 9)	(110 4)	(111 17)	(112 5)	(113 3)
(115 8)	(116 3)	(117 11)	(119 5)	(122 18)
(123 4)	(124 4)	(125 21)	(126 10)	(127 7)
(131 20)	(132 4)	(133 60)	(134 8)	(135 6)
(136 9)	(140 11)	(141 7)	(143 4)	(147 1000)
(148 161)	(149 97)	(150 10)	(151 3)	(153 7)
(155 6)	(157 12)	(168 10)	(169 30)	(170 7)
(171 4)	(184 10)	(185 37)	(186 6)	(196 3)
(197 5)	(212 73)	(213 22)	(214 5)	(215 5)
(258 3)	(259 9)	(286 4)	(287 81)	(288 19)
(289 7)	(302 2)			

NAME:12C\_1520.6\_1313EC75\_Aspartic acid (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:152002-10-1

RI:1521

RT:8.910

NUM PEAKS: 73

( 70 42)	( 71 9)	( 72 31)	( 73 1000)	( 74 107)
( 75 167)	( 77 8)	( 83 4)	( 85 5)	( 86 11)
( 87 6)	( 88 3)	( 89 4)	( 98 10)	(100 253)
(101 32)	(102 17)	(105 3)	(114 5)	(115 17)
(116 11)	(117 62)	(118 7)	(119 12)	(129 5)

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(130	29)	(131	23)	(132	19)	(133	56)	(134	10)
(135	6)	(142	17)	(143	7)	(144	9)	(145	3)
(146	5)	(147	167)	(148	29)	(149	27)	(150	3)
(158	3)	(160	9)	(161	3)	(163	17)	(164	3)
(172	9)	(173	3)	(174	14)	(175	3)	(177	4)
(188	45)	(189	11)	(190	7)	(202	46)	(203	9)
(204	13)	(205	4)	(216	21)	(217	7)	(218	80)
(220	6)	(221	4)	(231	6)	(232	382)	(233	80)
(234	38)	(244	4)	(245	4)	(246	3)	(292	5)
(306	11)	(307	3)	(334	5)				

NAME:12C\_1529.0\_1313EC75\_Pyroglutamic acid (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:153002-10-1

RI:1529

RT:8.976

NUM PEAKS: 63

( 70	20)	( 71	11)	( 72	45)	( 73	883)	( 74	81)
( 75	125)	( 76	8)	( 80	4)	( 82	6)	( 83	7)
( 84	28)	( 85	18)	( 86	24)	( 87	9)	( 88	3)
( 89	3)	( 94	3)	( 96	3)	( 97	3)	( 98	7)
( 99	9)	(100	17)	(101	5)	(102	5)	(103	8)
(105	3)	(110	5)	(112	25)	(113	8)	(114	14)
(115	8)	(117	10)	(119	3)	(122	3)	(126	3)
(129	4)	(131	19)	(132	5)	(133	35)	(134	5)
(135	3)	(140	28)	(141	10)	(142	8)	(147	160)
(148	26)	(149	16)	(154	9)	(155	6)	(156	1000)
(157	130)	(158	43)	(174	3)	(214	12)	(215	3)
(228	3)	(230	84)	(231	19)	(232	7)	(258	76)
(259	17)	(260	7)	(273	3)				

NAME:12C\_1659.6\_1313EC75\_[910; 2-Ketogluconic acid methoxyamine (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:166002-10-1

RI:1660

RT:9.991

NUM PEAKS: 40

( 72	21)	( 73	1000)	( 74	79)	( 75	73)	( 84	21)
( 87	8)	( 89	26)	(101	34)	(103	168)	(104	14)
(115	8)	(116	13)	(117	120)	(118	11)	(119	9)
(129	42)	(131	44)	(133	71)	(143	8)	(147	258)
(148	37)	(149	24)	(157	11)	(158	7)	(172	35)
(175	10)	(189	57)	(190	11)	(201	91)	(202	16)
(203	14)	(204	275)	(205	107)	(206	30)	(217	82)
(242	5)	(256	12)	(288	8)	(291	16)	(302	6)

NAME:12C\_1755.7\_1313EC75\_[829; Orotic acid (3TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:176003-10-1

RI:1756

RT:10.739

NUM PEAKS: 94

( 72	85)	( 73	1000)	( 78	4)	( 79	12)	( 80	8)
( 81	8)	( 83	17)	( 86	48)	( 91	8)	( 92	4)
( 93	9)	( 94	7)	( 97	21)	(100	165)	(102	9)
(104	3)	(105	7)	(106	5)	(107	4)	(108	3)
(109	3)	(119	8)	(120	5)	(123	6)	(124	4)
(131	66)	(132	15)	(133	66)	(134	10)	(135	7)
(137	4)	(147	214)	(148	35)	(149	20)	(156	10)
(158	15)	(160	9)	(161	5)	(167	9)	(174	77)

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(175	12)	(176	6)	(181	8)	(182	3)	(188	4)
(189	8)	(190	10)	(191	16)	(192	5)	(195	8)
(213	5)	(214	13)	(215	5)	(225	7)	(226	7)
(227	3)	(228	3)	(239	24)	(240	7)	(241	5)
(245	3)	(252	6)	(253	74)	(254	502)	(255	127)
(256	44)	(257	5)	(268	4)	(269	60)	(270	27)
(271	7)	(272	3)	(282	11)	(283	5)	(285	3)
(299	4)	(305	8)	(306	8)	(313	3)	(327	4)
(328	3)	(329	8)	(330	3)	(333	7)	(341	3)
(343	4)	(344	4)	(356	22)	(357	131)	(358	40)
(359	16)	(371	8)	(372	12)	(373	4)		

NAME:12C\_1758.1\_1313EC75\_[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:176005-10-1

RI:1758

RT:10.757

NUM PEAKS: 89

( 70	1000)	( 71	97)	( 72	22)	( 73	525)	( 74	109)
( 75	231)	( 76	21)	( 77	8)	( 80	3)	( 82	5)
( 83	20)	( 84	97)	( 85	186)	( 86	26)	( 87	17)
( 88	6)	( 90	23)	( 91	3)	( 95	47)	( 96	15)
( 97	8)	( 98	31)	( 99	122)	(100	32)	(101	21)
(102	10)	(103	26)	(104	3)	(110	5)	(111	5)
(112	9)	(113	18)	(114	14)	(115	27)	(116	28)
(117	20)	(118	4)	(122	5)	(124	3)	(125	30)
(126	18)	(127	37)	(128	10)	(129	25)	(130	53)
(131	27)	(132	10)	(139	9)	(140	24)	(141	54)
(143	15)	(144	20)	(145	7)	(146	7)	(147	30)
(148	6)	(149	5)	(151	3)	(152	4)	(154	8)
(155	13)	(156	5)	(157	19)	(158	5)	(159	27)
(160	4)	(167	9)	(168	39)	(169	12)	(170	10)
(171	10)	(172	82)	(173	16)	(183	18)	(184	416)
(185	65)	(186	55)	(187	21)	(188	4)	(196	5)
(211	9)	(212	3)	(229	4)	(258	11)	(259	3)
(284	3)	(285	3)	(286	8)	(301	3)		

NAME:12C\_1763.9\_1313EC75\_Ornithine (3TMS); Arginine (BP) (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:176006-10-1

RI:1764

RT:10.803

NUM PEAKS: 96

( 70	139)	( 71	16)	( 72	26)	( 73	1000)	( 74	173)
( 75	186)	( 76	17)	( 77	7)	( 80	9)	( 82	3)
( 83	5)	( 84	9)	( 85	10)	( 86	210)	( 87	38)
( 88	14)	( 90	15)	( 91	3)	( 96	9)	( 97	17)
( 98	15)	( 99	10)	(100	115)	(101	18)	(102	36)
(103	13)	(104	4)	(110	5)	(112	10)	(113	10)
(114	20)	(115	19)	(116	22)	(117	24)	(118	5)
(119	3)	(126	7)	(128	43)	(129	11)	(130	75)
(131	48)	(132	27)	(133	17)	(134	4)	(140	7)
(141	7)	(142	188)	(143	30)	(144	28)	(145	5)
(146	60)	(147	94)	(148	31)	(149	13)	(150	3)
(152	4)	(153	6)	(154	23)	(155	4)	(156	5)
(157	3)	(158	13)	(159	26)	(160	14)	(161	12)
(162	8)	(169	12)	(170	13)	(171	5)	(172	45)
(173	9)	(174	697)	(175	129)	(176	59)	(177	7)
(186	203)	(187	47)	(188	15)	(189	3)	(200	11)



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(201 3) (204 5) (213 3) (215 4) (216 33)  
(217 7) (218 4) (243 9) (244 62) (245 14)  
(246 5) (258 18) (259 7) (348 37) (349 12)  
(350 5)

NAME:12C\_1769.9\_1313EC75\_Glycerol-3-phosphate (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:177002-10-1

RI:1770

RT:10.850

NUM PEAKS: 108

( 71 7) ( 72 27) ( 73 1000) ( 74 86) ( 77 15)  
( 85 7) ( 88 6) ( 91 5) ( 99 6) (101 102)  
(103 118) (104 12) (105 12) (107 5) (113 20)  
(115 23) (116 25) (117 24) (119 13) (121 7)  
(123 3) (129 69) (131 56) (132 8) (133 113)  
(134 15) (135 33) (136 4) (137 13) (139 3)  
(147 155) (148 23) (149 21) (150 3) (151 9)  
(153 3) (163 8) (165 4) (177 3) (179 4)  
(181 17) (182 3) (183 8) (191 16) (193 20)  
(194 4) (195 18) (196 3) (197 6) (203 11)  
(205 8) (207 32) (208 7) (209 6) (210 3)  
(211 93) (212 17) (213 11) (220 3) (225 20)  
(226 6) (227 18) (228 3) (241 17) (242 4)  
(243 10) (253 6) (255 4) (256 19) (269 6)  
(283 6) (284 3) (285 19) (286 5) (287 3)  
(298 18) (299 175) (300 47) (301 25) (302 5)  
(313 4) (314 11) (315 42) (316 12) (317 6)  
(327 4) (328 9) (341 14) (342 7) (343 3)  
(356 18) (357 112) (358 34) (359 16) (360 3)  
(369 3) (370 21) (371 7) (372 4) (373 9)  
(374 3) (386 3) (387 12) (388 5) (389 5)  
(444 4) (445 17) (446 7)

NAME:12C\_1802.0\_1313EC75\_[706; Xylitol (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:180002-10-1

RI:1802

RT:11.098

NUM PEAKS: 69

( 72 14) ( 73 1000) ( 74 101) ( 75 140) ( 87 4)  
( 88 4) ( 89 11) (100 4) (101 12) (102 11)  
(103 34) (104 6) (113 5) (115 6) (116 8)  
(117 40) (118 6) (119 5) (128 13) (129 50)  
(130 10) (131 19) (132 5) (133 35) (134 5)  
(135 4) (141 21) (142 6) (143 19) (144 10)  
(145 3) (147 141) (148 21) (149 19) (155 5)  
(157 23) (169 9) (189 20) (190 4) (191 33)  
(192 5) (203 3) (205 16) (206 3) (215 9)  
(217 54) (218 13) (219 11) (220 3) (221 7)  
(229 8) (230 6) (231 7) (232 4) (243 3)  
(245 3) (246 4) (257 39) (258 10) (259 4)  
(272 4) (303 6) (319 6) (347 5) (362 3)  
(436 5) (437 23) (438 11) (439 5)

NAME:12C\_1813.0\_1313EC75\_Glyceric acid-3-phosphate (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:181003-10-1

RI:1813

RT:11.184

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NUM PEAKS: 69

( 72	28)	( 73	1000)	( 74	80)	( 75	112)	( 77	20)
( 87	9)	( 89	17)	( 90	5)	(101	87)	(102	11)
(104	7)	(105	13)	(107	6)	(115	16)	(116	29)
(117	17)	(121	10)	(132	8)	(133	101)	(134	16)
(135	32)	(137	15)	(141	4)	(144	6)	(147	252)
(148	39)	(149	26)	(151	11)	(153	5)	(181	19)
(189	15)	(190	5)	(193	19)	(194	5)	(195	18)
(207	28)	(211	118)	(212	20)	(213	12)	(214	5)
(225	19)	(226	7)	(227	99)	(228	17)	(229	9)
(243	5)	(298	12)	(299	125)	(300	36)	(301	17)
(302	3)	(315	45)	(316	14)	(317	8)	(341	11)
(342	6)	(343	6)	(352	3)	(356	14)	(357	66)
(358	20)	(359	8)	(386	10)	(387	32)	(388	14)
(389	8)	(458	6)	(459	13)	(460	6)		

NAME:12C\_1819.8\_1313EC75\_Ornithine (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:182002-10-1

RI:1820

RT:11.237

NUM PEAKS: 105

( 70	24)	( 71	9)	( 72	19)	( 73	1000)	( 74	117)
( 80	3)	( 82	3)	( 83	4)	( 84	12)	( 85	10)
( 86	112)	( 87	16)	( 88	7)	( 90	5)	( 91	3)
( 96	5)	( 98	14)	(100	104)	(101	18)	(102	46)
(103	19)	(104	4)	(110	9)	(112	17)	(113	9)
(114	31)	(115	23)	(116	16)	(117	19)	(118	5)
(119	6)	(124	3)	(126	19)	(127	13)	(128	53)
(130	59)	(131	31)	(132	29)	(133	26)	(134	6)
(140	12)	(141	12)	(142	898)	(143	127)	(144	49)
(145	6)	(146	41)	(152	7)	(153	4)	(154	6)
(156	4)	(158	9)	(159	6)	(160	12)	(161	5)
(162	4)	(168	4)	(169	10)	(170	6)	(172	38)
(173	9)	(174	294)	(175	54)	(176	29)	(177	4)
(186	13)	(187	12)	(188	9)	(189	15)	(190	5)
(191	7)	(198	3)	(200	57)	(201	14)	(202	10)
(203	8)	(204	19)	(205	5)	(214	30)	(215	10)
(216	33)	(217	12)	(218	17)	(219	4)	(220	5)
(226	3)	(230	4)	(232	4)	(241	6)	(242	4)
(243	3)	(244	6)	(258	21)	(259	21)	(260	6)
(303	4)	(315	5)	(316	3)	(330	7)	(331	3)
(405	3)	(419	3)	(420	15)	(421	7)	(422	4)

NAME:12C\_1827.9\_1313EC75\_Arginine (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:183001-10-1

RI:1828

RT:11.300

NUM PEAKS: 43

( 70	162)	( 71	26)	( 73	1000)	( 74	25)	( 84	87)
( 85	30)	( 98	17)	(100	88)	(112	7)	(114	17)
(115	41)	(125	7)	(126	5)	(127	21)	(128	15)
(130	10)	(132	15)	(140	41)	(141	122)	(142	239)
(143	17)	(155	25)	(156	26)	(157	667)	(158	83)
(167	9)	(168	14)	(171	25)	(172	33)	(173	5)
(187	13)	(188	7)	(215	7)	(216	13)	(240	10)
(244	15)	(256	223)	(257	50)	(258	15)	(292	3)
(358	4)	(371	2)	(373	5)				

NAME:12C\_1835.3\_1313EC75\_[731; Erythrose (3TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:184003-10-1

RI:1835

RT:11.358

NUM PEAKS: 137

( 70	8)	( 71	7)	( 72	22)	( 73	1000)	( 74	89)
( 75	143)	( 76	9)	( 77	11)	( 80	4)	( 81	3)
( 82	6)	( 83	37)	( 84	87)	( 85	15)	( 86	5)
( 87	12)	( 88	6)	( 89	43)	( 90	4)	( 91	3)
( 94	3)	( 96	12)	( 97	4)	( 98	4)	( 99	15)
(100	21)	(101	33)	(102	9)	(103	93)	(104	10)
(108	6)	(109	3)	(110	3)	(111	10)	(112	4)
(113	26)	(114	11)	(115	25)	(116	32)	(117	131)
(118	14)	(119	14)	(122	3)	(124	3)	(126	3)
(127	5)	(128	20)	(129	84)	(130	18)	(131	42)
(132	10)	(133	74)	(134	11)	(135	10)	(136	6)
(141	4)	(142	7)	(143	22)	(144	13)	(145	7)
(146	3)	(147	250)	(148	40)	(149	47)	(150	10)
(151	3)	(152	3)	(155	4)	(156	45)	(157	22)
(158	12)	(159	27)	(163	20)	(164	4)	(168	12)
(173	29)	(174	8)	(175	7)	(177	10)	(182	11)
(183	4)	(184	12)	(185	4)	(186	4)	(189	45)
(190	11)	(191	75)	(192	13)	(193	6)	(196	7)
(197	5)	(198	23)	(199	4)	(200	3)	(201	5)
(202	17)	(203	42)	(204	68)	(205	21)	(206	7)
(207	3)	(210	9)	(211	6)	(215	8)	(216	4)
(217	103)	(218	89)	(219	23)	(220	7)	(221	3)
(224	7)	(226	54)	(227	9)	(228	3)	(229	3)
(230	10)	(231	43)	(232	11)	(233	24)	(234	5)
(239	6)	(240	3)	(245	3)	(246	8)	(258	4)
(272	5)	(300	10)	(301	3)	(314	5)	(316	7)
(317	3)	(318	10)	(319	6)	(320	3)	(329	24)
(330	7)	(404	5)						

NAME:12C\_1869.1\_1313EC75\_Fructose methoxyamine (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:187002-10-1

RI:1869

RT:11.621

NUM PEAKS: 87

( 70	5)	( 71	5)	( 72	19)	( 73	1000)	( 74	83)
( 75	63)	( 76	3)	( 82	4)	( 84	16)	( 85	5)
( 87	7)	( 88	6)	( 89	47)	( 90	4)	( 99	4)
(100	10)	(101	17)	(102	5)	(103	351)	(104	35)
(105	17)	(113	4)	(114	8)	(115	7)	(116	5)
(117	54)	(118	6)	(119	8)	(126	3)	(128	3)
(129	40)	(130	8)	(131	22)	(132	4)	(133	71)
(134	9)	(135	5)	(142	5)	(143	8)	(145	5)
(147	183)	(148	30)	(149	19)	(157	7)	(158	3)
(159	3)	(163	8)	(172	14)	(173	17)	(174	4)
(175	6)	(177	4)	(189	30)	(190	7)	(191	16)
(192	3)	(201	8)	(202	6)	(203	4)	(204	14)
(205	22)	(206	5)	(207	5)	(214	3)	(216	5)
(217	222)	(218	46)	(219	22)	(220	3)	(221	6)
(231	6)	(244	3)	(256	3)	(260	3)	(262	4)
(263	6)	(277	17)	(278	6)	(279	3)	(291	4)
(306	3)	(307	76)	(308	23)	(309	11)	(335	5)
(364	11)	(365	4)						

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NAME:12C\_1879.6\_1313EC75\_Fructose methoxyamine (BP) (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:188004-10-1

RI:1880

RT:11.703

NUM PEAKS: 81

( 70	6)	( 71	5)	( 72	19)	( 73	1000)	( 74	88)
( 75	78)	( 82	7)	( 84	35)	( 85	7)	( 86	4)
( 87	8)	( 88	6)	( 89	72)	( 90	6)	( 99	4)
(100	12)	(101	21)	(102	5)	(103	365)	(104	38)
(105	26)	(113	6)	(114	26)	(115	9)	(116	8)
(117	55)	(118	7)	(119	11)	(126	3)	(128	4)
(129	40)	(133	59)	(134	8)	(135	5)	(142	7)
(143	9)	(145	6)	(147	216)	(148	35)	(156	3)
(159	3)	(172	9)	(173	17)	(175	7)	(177	3)
(188	3)	(189	29)	(190	7)	(191	18)	(192	3)
(198	3)	(201	7)	(202	8)	(203	5)	(204	16)
(205	28)	(206	6)	(207	5)	(216	5)	(217	255)
(218	55)	(219	25)	(221	7)	(231	6)	(244	6)
(245	3)	(262	14)	(263	9)	(264	3)	(277	18)
(278	6)	(279	3)	(291	3)	(306	4)	(307	86)
(308	26)	(309	12)	(335	5)	(336	3)	(364	12)
(365	4)								

NAME:12C\_1931.9\_1313EC75\_Sorbitol (6TMS); Glucitol (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:193001-10-1

RI:1932

RT:12.063

NUM PEAKS: 90

( 70	3)	( 71	4)	( 72	19)	( 73	1000)	( 74	88)
( 75	66)	( 76	3)	( 81	3)	( 83	10)	( 85	4)
( 87	8)	( 88	5)	( 89	26)	( 90	3)	( 97	6)
( 99	4)	(101	24)	(102	5)	(103	175)	(104	17)
(105	9)	(111	3)	(113	5)	(115	7)	(116	7)
(117	100)	(118	10)	(119	8)	(127	3)	(129	83)
(130	10)	(131	27)	(132	4)	(133	59)	(134	8)
(135	6)	(141	3)	(143	14)	(145	4)	(147	316)
(148	51)	(149	33)	(150	4)	(155	4)	(157	60)
(158	8)	(159	5)	(163	5)	(169	4)	(175	9)
(177	5)	(183	7)	(189	34)	(190	9)	(191	32)
(192	6)	(193	3)	(203	5)	(204	41)	(205	148)
(206	30)	(207	15)	(217	153)	(218	32)	(219	14)
(220	3)	(221	9)	(229	15)	(230	6)	(231	16)
(232	4)	(255	6)	(259	4)	(277	7)	(278	4)
(291	7)	(305	8)	(306	5)	(307	24)	(308	7)
(309	3)	(318	7)	(319	118)	(320	38)	(321	17)
(322	4)	(331	8)	(332	3)	(345	5)	(421	3)

NAME:12C\_1956.6\_1313EC75\_[793; D-Galactono-1,4-lactone (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:196004-10-1

RI:1957

RT:12.219

NUM PEAKS: 124

( 70	11)	( 71	5)	( 72	20)	( 73	1000)	( 74	85)
( 75	117)	( 76	10)	( 77	8)	( 81	12)	( 82	17)
( 83	5)	( 85	6)	( 86	4)	( 87	7)	( 88	5)
( 89	50)	( 90	5)	( 91	6)	( 96	3)	( 97	4)
( 98	3)	( 99	7)	(100	11)	(101	24)	(102	11)

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(103	101)	(104	11)	(105	14)	(109	5)	(110	5)
(111	7)	(112	3)	(113	5)	(114	5)	(115	11)
(116	11)	(117	54)	(118	7)	(119	10)	(126	4)
(127	5)	(128	5)	(129	88)	(130	30)	(131	31)
(132	7)	(133	56)	(134	8)	(135	6)	(139	3)
(141	3)	(142	12)	(143	18)	(144	5)	(145	8)
(146	4)	(147	165)	(148	48)	(149	26)	(150	4)
(153	4)	(154	3)	(155	12)	(156	4)	(157	29)
(158	12)	(159	5)	(160	15)	(161	14)	(162	3)
(163	10)	(168	4)	(169	55)	(170	34)	(171	9)
(172	4)	(173	4)	(174	8)	(177	3)	(183	4)
(186	9)	(189	34)	(190	8)	(191	21)	(192	4)
(200	3)	(201	3)	(203	7)	(204	48)	(205	21)
(206	6)	(207	3)	(215	4)	(216	5)	(217	218)
(218	47)	(219	31)	(220	5)	(221	4)	(228	3)
(229	7)	(230	4)	(231	6)	(232	3)	(242	6)
(243	28)	(244	13)	(245	8)	(246	4)	(247	4)
(248	3)	(259	3)	(260	4)	(271	18)	(272	5)
(273	3)	(291	3)	(331	5)	(332	13)	(333	5)
(360	4)	(361	43)	(362	15)	(363	7)		

NAME:12C\_1999.3\_1313EC75\_Gluconic acid (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:200001-10-1

RI:1999

RT:12.490

NUM PEAKS: 87

( 72	18)	( 73	1000)	( 74	88)	( 75	67)	( 76	3)
( 81	7)	( 82	8)	( 83	28)	( 84	8)	( 85	10)
( 89	14)	( 96	5)	( 97	26)	( 98	5)	(101	15)
(102	14)	(103	98)	(104	9)	(105	6)	(111	12)
(113	4)	(115	4)	(117	56)	(118	6)	(119	7)
(125	6)	(129	48)	(130	12)	(131	27)	(132	4)
(133	53)	(134	7)	(135	6)	(143	30)	(144	3)
(145	3)	(147	310)	(148	49)	(149	31)	(150	3)
(153	3)	(157	19)	(161	3)	(169	5)	(171	6)
(175	5)	(189	32)	(190	9)	(191	18)	(204	32)
(205	58)	(206	12)	(207	10)	(217	66)	(218	14)
(219	12)	(220	4)	(221	14)	(222	3)	(229	7)
(230	3)	(231	4)	(245	5)	(277	10)	(278	3)
(291	8)	(292	59)	(293	18)	(294	8)	(305	25)
(306	9)	(307	8)	(318	3)	(319	27)	(320	9)
(331	4)	(332	7)	(333	55)	(334	18)	(335	8)
(345	3)	(359	8)	(360	3)	(423	6)	(433	3)
(434	3)	(435	4)						

NAME:12C\_2048.2\_1313EC75\_Hexadecanoic acid (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:205001-10-1

RI:2048

RT:12.799

NUM PEAKS: 111

( 70	27)	( 71	43)	( 72	51)	( 73	944)	( 74	111)
( 75	1000)	( 76	74)	( 77	54)	( 79	26)	( 80	4)
( 81	70)	( 82	10)	( 83	74)	( 84	29)	( 85	30)
( 86	14)	( 87	11)	( 88	8)	( 89	29)	( 90	5)
( 91	11)	( 93	23)	( 94	4)	( 95	65)	( 96	10)
( 97	54)	( 98	41)	( 99	27)	(100	5)	(101	17)
(102	6)	(105	29)	(106	3)	(107	12)	(109	19)
(110	4)	(111	25)	(112	12)	(113	6)	(115	10)

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(116	67)	(117	969)	(118	95)	(119	41)	(121	9)
(123	6)	(125	7)	(126	5)	(127	5)	(128	4)
(129	492)	(130	64)	(131	174)	(132	459)	(133	90)
(134	22)	(135	9)	(137	3)	(139	5)	(140	5)
(141	4)	(142	4)	(143	45)	(144	7)	(145	233)
(146	31)	(153	5)	(154	7)	(155	6)	(157	15)
(158	4)	(159	26)	(167	3)	(168	3)	(171	24)
(172	4)	(173	8)	(174	6)	(185	33)	(186	5)
(187	21)	(188	6)	(195	4)	(199	10)	(201	53)
(202	10)	(203	3)	(213	10)	(214	3)	(215	8)
(216	3)	(227	11)	(228	3)	(229	12)	(230	3)
(241	5)	(243	12)	(244	3)	(257	7)	(269	15)
(270	4)	(271	4)	(283	3)	(285	15)	(286	4)
(312	15)	(313	233)	(314	66)	(315	17)	(328	26)
(329	8)								

NAME:12C\_2087.4\_1313EC75\_[756; beta-D-Methylglucopyranoside (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:209004-10-1

RI:2087

RT:13.047

NUM PEAKS: 68

( 70	6)	( 72	21)	( 73	1000)	( 74	88)	( 75	70)
( 81	6)	( 82	6)	( 83	7)	( 86	6)	( 88	3)
( 89	78)	( 90	7)	( 97	4)	(100	42)	(101	34)
(102	16)	(103	61)	(105	11)	(115	8)	(116	15)
(117	36)	(118	4)	(129	57)	(130	10)	(131	27)
(132	12)	(133	44)	(134	7)	(135	6)	(142	5)
(143	13)	(145	7)	(147	212)	(148	60)	(149	28)
(155	5)	(157	30)	(160	9)	(161	5)	(163	8)
(169	8)	(172	10)	(187	3)	(189	31)	(190	9)
(201	5)	(203	12)	(204	342)	(205	83)	(206	32)
(207	8)	(216	3)	(217	56)	(218	16)	(219	8)
(220	69)	(221	18)	(222	6)	(229	6)	(230	5)
(231	8)	(233	10)	(243	8)	(244	5)	(247	3)
(319	64)	(320	23)	(321	11)				

NAME:12C\_2064.0\_1191EC10\_[770; 3,4,6-Trishydroxyphenylethanolamine (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:206001-10-1

RI:2064

RT:13.339

NUM PEAKS: 191

( 70	28)	( 71	17)	( 72	20)	( 75	211)	( 77	38)
( 81	37)	( 82	17)	( 83	13)	( 86	301)	( 87	27)
( 88	5)	( 90	3)	( 91	11)	( 93	24)	( 95	10)
( 96	4)	( 98	7)	(100	150)	(101	32)	(102	84)
(105	5)	(106	4)	(107	6)	(109	20)	(112	6)
(113	9)	(114	12)	(115	15)	(116	15)	(117	181)
(118	16)	(119	11)	(121	7)	(122	4)	(123	14)
(124	3)	(125	9)	(128	8)	(130	62)	(131	20)
(132	25)	(133	44)	(134	5)	(135	6)	(136	7)
(137	4)	(139	4)	(142	13)	(143	10)	(144	13)
(146	19)	(147	61)	(148	15)	(149	16)	(150	4)
(151	4)	(156	5)	(157	7)	(158	34)	(161	3)
(162	6)	(164	5)	(170	6)	(171	12)	(172	37)
(173	5)	(174	1000)	(175	168)	(176	129)	(177	15)
(182	6)	(186	8)	(187	14)	(188	10)	(189	6)
(191	11)	(196	5)	(199	6)	(200	9)	(201	5)
(202	8)	(203	4)	(204	16)	(207	9)	(208	7)

153

(211	8)	(213	5)	(217	8)	(220	8)	(226	4)
(227	13)	(233	7)	(234	3)	(235	3)	(243	6)
(244	4)	(246	3)	(248	8)	(250	3)	(252	9)
(257	13)	(258	8)	(259	9)	(261	6)	(262	3)
(264	8)	(266	11)	(269	6)	(270	3)	(271	3)
(275	8)	(276	6)	(284	5)	(285	7)	(290	3)
(291	3)	(301	3)	(303	5)	(307	3)	(309	4)
(310	4)	(311	3)	(313	5)	(317	5)	(321	7)
(322	5)	(333	8)	(334	4)	(335	5)	(337	3)
(338	6)	(339	3)	(343	3)	(344	4)	(345	3)
(346	3)	(347	4)	(348	10)	(353	3)	(354	3)
(359	8)	(361	8)	(365	4)	(367	3)	(376	3)
(377	5)	(378	4)	(389	4)	(390	6)	(392	5)
(395	5)	(411	4)	(420	6)	(421	4)	(424	5)
(425	3)	(428	3)	(435	3)	(448	13)	(449	47)
(450	26)	(451	18)	(466	6)	(467	3)	(469	4)
(470	5)	(473	3)	(475	4)	(478	4)	(484	3)
(488	5)	(493	3)	(495	5)	(498	7)	(500	5)
(507	3)	(512	4)	(514	5)	(515	6)	(525	3)
(529	5)	(530	3)	(533	6)	(534	8)	(543	6)
(547	5)	(553	4)	(557	4)	(567	3)	(575	3)
(595	4)								

NAME:12C\_2023.2\_1160EC43\_[766; beta-D-Methylglucopyranoside (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:203003-10-1

RI:2023

RT:13.133

NUM PEAKS: 92

( 70	4)	( 71	3)	( 72	17)	( 73	1000)	( 74	84)
( 75	90)	( 76	5)	( 77	5)	( 81	5)	( 83	4)
( 84	7)	( 85	4)	( 86	3)	( 87	4)	( 88	3)
( 89	75)	( 90	7)	( 91	7)	( 97	4)	( 99	5)
(100	46)	(101	23)	(102	17)	(103	75)	(104	8)
(105	10)	(111	3)	(113	6)	(115	9)	(116	12)
(117	34)	(118	4)	(119	7)	(127	3)	(128	4)
(129	68)	(130	13)	(131	26)	(132	12)	(133	48)
(134	6)	(135	4)	(142	5)	(143	15)	(144	3)
(145	6)	(147	176)	(148	57)	(149	25)	(150	3)
(155	4)	(157	32)	(158	6)	(159	4)	(160	7)
(161	5)	(163	7)	(169	9)	(170	3)	(172	8)
(173	3)	(174	3)	(175	3)	(177	3)	(189	36)
(190	10)	(191	22)	(192	4)	(203	8)	(204	398)
(205	97)	(206	38)	(207	8)	(217	85)	(218	23)
(219	10)	(220	80)	(221	18)	(222	7)	(229	5)
(230	5)	(231	6)	(233	13)	(234	3)	(243	9)
(244	4)	(259	6)	(291	3)	(305	4)	(319	69)
(320	23)	(321	11)						

NAME:12C\_2002.2\_1178EC16\_[775; Dopamine (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:200002-10-1

RI:2002

RT:12.973

NUM PEAKS: 186

( 70	70)	( 72	16)	( 73	932)	( 74	101)	( 75	182)
( 76	10)	( 77	8)	( 80	10)	( 82	14)	( 84	13)
( 86	211)	( 87	27)	( 88	6)	( 89	6)	( 90	4)
( 94	28)	( 95	3)	( 96	11)	( 98	21)	( 99	5)
(100	103)	(101	17)	(102	32)	(103	14)	(104	5)

154

(105	5)	(106	4)	(110	4)	(111	7)	(112	23)
(113	6)	(114	19)	(115	15)	(116	42)	(117	19)
(118	7)	(119	5)	(121	5)	(122	3)	(123	3)
(126	5)	(128	29)	(129	9)	(130	74)	(131	41)
(132	16)	(133	30)	(134	7)	(135	7)	(138	3)
(139	9)	(140	7)	(141	3)	(142	107)	(143	21)
(144	17)	(146	31)	(147	77)	(148	16)	(149	20)
(150	7)	(151	4)	(152	9)	(153	3)	(154	8)
(156	11)	(158	13)	(159	5)	(160	4)	(161	5)
(163	4)	(166	4)	(168	9)	(169	4)	(170	24)
(171	14)	(172	28)	(173	18)	(174	1000)	(175	174)
(176	77)	(177	9)	(184	12)	(186	44)	(187	7)
(188	5)	(190	4)	(195	4)	(196	4)	(199	3)
(200	19)	(201	6)	(202	5)	(203	3)	(204	3)
(206	3)	(208	3)	(209	3)	(211	10)	(212	3)
(213	4)	(214	45)	(215	10)	(216	12)	(220	3)
(221	3)	(222	4)	(227	6)	(228	14)	(229	7)
(230	8)	(231	3)	(232	3)	(244	7)	(246	3)
(252	3)	(258	6)	(260	3)	(261	20)	(262	6)
(263	3)	(270	3)	(272	3)	(274	3)	(281	3)
(285	6)	(286	7)	(287	4)	(289	8)	(298	3)
(301	5)	(303	3)	(314	3)	(317	34)	(318	13)
(319	4)	(320	3)	(323	3)	(331	3)	(332	3)
(344	3)	(352	3)	(353	3)	(357	4)	(362	3)
(375	23)	(376	9)	(377	7)	(378	3)	(388	3)
(389	5)	(390	6)	(395	3)	(397	3)	(403	4)
(404	3)	(408	3)	(413	3)	(415	3)	(425	3)
(429	3)	(432	3)	(433	3)	(436	3)	(440	3)
(444	3)	(455	3)	(461	3)	(466	3)	(467	4)
(480	4)	(481	4)	(491	3)	(502	4)	(503	3)
(514	5)	(517	3)	(522	4)	(523	3)	(526	3)
(528	3)	(535	3)	(547	3)	(549	4)	(550	3)
(551	4)								

NAME:12C\_1882.5\_1274EC11\_Mannose methoxyamine (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:188002-10-1

RI:1883

RT:12.225

NUM PEAKS: 114

( 72	6)	( 73	1000)	( 74	78)	( 75	158)	( 76	43)
( 77	12)	( 81	6)	( 85	3)	( 87	3)	( 88	5)
( 89	36)	( 90	3)	( 91	9)	( 93	19)	( 94	4)
( 97	5)	( 99	10)	(100	10)	(101	28)	(102	11)
(103	139)	(104	47)	(105	32)	(106	7)	(111	3)
(113	5)	(115	11)	(116	17)	(117	114)	(118	13)
(119	16)	(120	3)	(121	16)	(122	7)	(123	6)
(126	6)	(127	5)	(129	183)	(130	32)	(131	43)
(132	15)	(134	3)	(135	8)	(138	5)	(141	3)
(142	8)	(143	24)	(144	5)	(145	10)	(147	118)
(148	19)	(151	7)	(154	4)	(155	4)	(156	3)
(157	138)	(158	23)	(159	11)	(163	26)	(164	4)
(167	20)	(168	4)	(169	13)	(170	4)	(171	7)
(173	42)	(174	26)	(175	7)	(177	5)	(182	3)
(186	9)	(187	4)	(189	87)	(190	18)	(196	3)
(197	3)	(201	4)	(203	8)	(205	126)	(206	21)
(207	11)	(214	5)	(215	6)	(217	100)	(218	18)
(219	23)	(220	48)	(221	14)	(222	6)	(223	28)
(224	4)	(229	24)	(230	9)	(231	7)	(243	16)
(244	12)	(245	8)	(246	4)	(247	20)	(248	6)



155

(249 3) (257 3) (259 5) (271 4) (277 3)  
 (302 4) (304 5) (305 4) (306 3) (319 53)  
 (320 14) (321 6) (333 8) (334 3)

NAME:12C\_1882.4\_1160EC15\_Adenine (2TMS)  
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
 CASNO:188005-10-1  
 RI:1882  
 RT:12.217

NUM PEAKS: 37

( 73 675) ( 79 56) ( 81 27) ( 84 169) ( 86 45)  
 ( 91 126) ( 95 59) ( 99 74) (103 15) (109 161)  
 (110 61) (115 31) (117 21) (119 79) (120 56)  
 (122 30) (137 34) (164 22) (165 80) (167 56)  
 (176 17) (192 219) (193 42) (227 138) (264 1000)  
 (265 190) (266 43) (270 9) (278 128) (279 206)  
 (359 9) (413 24) (431 24) (462 10) (484 19)  
 (500 12) (582 25)

NAME:12C\_1850.9\_1274EC11\_[912; Tetradecanoic acid (1TMS)]  
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
 CASNO:185004-10-1  
 RI:1851

RT:11.982

NUM PEAKS: 82

( 70 17) ( 71 20) ( 72 43) ( 73 681) ( 74 70)  
 ( 75 933) ( 76 67) ( 77 47) ( 79 19) ( 81 57)  
 ( 83 42) ( 85 16) ( 87 5) ( 89 21) ( 90 4)  
 ( 91 7) ( 93 15) ( 95 52) ( 96 7) ( 97 34)  
 ( 98 31) ( 99 19) (101 11) (105 29) (107 8)  
 (109 16) (111 17) (112 8) (115 6) (116 62)  
 (117 1000) (118 99) (119 40) (121 6) (123 4)  
 (125 5) (129 412) (130 43) (131 178) (132 449)  
 (133 86) (134 22) (135 5) (141 3) (143 37)  
 (144 3) (145 203) (146 24) (147 8) (153 3)  
 (154 7) (155 3) (159 26) (167 5) (171 18)  
 (173 8) (185 23) (186 3) (187 16) (188 4)  
 (199 7) (201 49) (202 8) (203 3) (204 3)  
 (213 9) (215 10) (216 3) (227 6) (229 3)  
 (241 16) (242 4) (243 7) (257 19) (284 3)  
 (285 222) (286 55) (287 15) (299 9) (300 30)  
 (301 8) (302 3)

NAME:12C\_1822.5\_1313EC75\_Citric acid (4TMS)  
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
 CASNO:182004-10-1  
 RI:1823

RT:11.258

NUM PEAKS: 87

( 70 7) ( 71 5) ( 72 35) ( 73 1000) ( 74 85)  
 ( 75 185) ( 76 12) ( 77 22) ( 79 3) ( 83 3)  
 ( 85 3) ( 87 4) ( 88 3) ( 95 5) ( 97 7)  
 ( 99 17) (101 6) (111 9) (115 18) (116 9)  
 (117 15) (118 3) (119 5) (129 25) (130 3)  
 (131 28) (132 4) (133 46) (134 7) (135 6)  
 (139 5) (141 8) (142 3) (143 17) (145 3)  
 (147 288) (148 46) (149 48) (150 6) (151 4)  
 (157 6) (163 5) (169 5) (171 6) (183 39)  
 (184 6) (185 11) (189 4) (190 4) (191 5)  
 (201 3) (207 7) (211 46) (212 7) (213 8)

156

(215	7)	(217	10)	(221	20)	(222	5)	(223	3)
(229	5)	(231	11)	(232	3)	(245	3)	(257	23)
(258	6)	(259	5)	(273	171)	(274	39)	(275	17)
(285	6)	(301	4)	(303	5)	(305	10)	(306	3)
(347	32)	(348	11)	(349	6)	(363	22)	(364	7)
(365	3)	(375	26)	(376	9)	(377	5)	(465	9)
(466	5)	(467	3)						

NAME:12C\_1824.3\_1191EC08\_[570; Hypoxanthine (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:182006-10-1

RI:1824

RT:11.718

NUM PEAKS: 163

( 71	177)	( 74	499)	( 79	33)	( 80	60)	( 81	31)
( 85	268)	( 86	997)	( 90	10)	( 91	279)	( 98	29)
( 99	87)	(100	809)	(102	373)	(104	78)	(105	781)
(106	124)	(107	7)	(108	8)	(109	35)	(110	55)
(111	29)	(112	89)	(113	12)	(114	40)	(118	70)
(119	103)	(120	56)	(121	30)	(123	111)	(124	55)
(125	151)	(126	50)	(138	29)	(140	57)	(144	25)
(145	61)	(152	36)	(154	61)	(159	15)	(165	9)
(166	101)	(170	15)	(172	118)	(173	82)	(178	19)
(179	15)	(180	23)	(181	81)	(182	30)	(184	19)
(187	16)	(188	70)	(190	16)	(191	58)	(192	55)
(193	99)	(194	22)	(195	10)	(197	22)	(198	25)
(199	33)	(201	48)	(202	16)	(203	19)	(204	24)
(205	31)	(206	153)	(207	8)	(208	22)	(214	33)
(215	18)	(219	19)	(220	25)	(226	21)	(227	6)
(229	99)	(230	32)	(234	21)	(238	30)	(239	24)
(241	308)	(242	128)	(243	31)	(244	21)	(248	9)
(249	26)	(250	17)	(251	10)	(252	20)	(253	4)
(254	6)	(258	222)	(259	82)	(260	14)	(261	8)
(262	11)	(263	10)	(264	20)	(265	1000)	(266	253)
(267	101)	(270	31)	(277	9)	(279	32)	(280	326)
(281	86)	(282	17)	(288	12)	(289	10)	(303	5)
(304	10)	(315	8)	(316	16)	(317	4)	(326	4)
(329	22)	(330	19)	(331	25)	(332	25)	(337	5)
(341	10)	(343	11)	(351	15)	(356	3)	(357	9)
(378	4)	(388	3)	(403	7)	(405	12)	(406	19)
(407	7)	(421	10)	(422	18)	(423	26)	(424	3)
(431	6)	(435	4)	(439	4)	(445	8)	(446	6)
(450	6)	(451	4)	(458	8)	(462	11)	(469	7)
(471	3)	(476	4)	(501	7)	(524	5)	(529	4)
(530	6)	(537	4)	(538	6)	(543	4)	(561	6)
(564	3)	(568	8)	(569	7)	(571	6)	(575	4)
(581	4)	(582	3)	(595	3)				

NAME:12C\_1771.1\_1274EC11\_[812; D-Xylofuranose (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:177004-10-1

RI:1771

RT:11.367

NUM PEAKS: 78

( 70	6)	( 72	13)	( 73	1000)	( 74	81)	( 75	94)
( 76	4)	( 77	5)	( 79	3)	( 81	10)	( 83	6)
( 84	6)	( 85	3)	( 87	4)	( 89	5)	( 95	4)
( 97	4)	( 99	7)	(103	12)	(109	4)	(111	5)
(113	5)	(115	4)	(116	4)	(117	30)	(118	3)
(119	6)	(127	4)	(128	3)	(129	28)	(130	3)

157

(131	11)	(133	47)	(141	4)	(142	7)	(143	19)
(144	7)	(145	6)	(147	226)	(148	35)	(149	35)
(150	4)	(155	5)	(157	7)	(159	6)	(161	3)
(163	9)	(169	20)	(170	4)	(171	3)	(177	4)
(189	5)	(191	38)	(203	15)	(204	5)	(205	3)
(215	3)	(217	523)	(218	137)	(219	55)	(220	9)
(221	5)	(231	5)	(232	56)	(233	15)	(234	6)
(243	6)	(245	6)	(255	3)	(257	16)	(258	4)
(271	4)	(305	16)	(306	5)	(307	3)	(318	3)
(450	18)	(451	10)	(452	5)				

NAME:12C\_1710.6\_1274EC17\_[817; Ribitol (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1711 |RI:1711

CASNO:171008-10-1

RI:1711

RT:10.896

SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp

NUM PEAKS: 148

( 72	16)	( 73	1000)	( 74	86)	( 75	260)	( 76	15)
( 77	32)	( 81	6)	( 83	29)	( 88	7)	( 89	11)
( 95	16)	( 97	26)	(101	105)	(102	14)	(103	209)
(104	22)	(105	11)	(109	13)	(110	8)	(114	6)
(116	41)	(117	114)	(118	12)	(119	15)	(121	11)
(122	8)	(129	164)	(130	27)	(133	88)	(134	10)
(136	6)	(137	8)	(138	25)	(139	35)	(140	13)
(143	14)	(144	6)	(145	11)	(147	428)	(148	69)
(149	84)	(150	14)	(156	4)	(157	35)	(163	21)
(164	9)	(169	34)	(170	7)	(171	5)	(175	7)
(177	6)	(185	11)	(186	8)	(187	36)	(188	11)
(189	35)	(190	11)	(191	29)	(192	7)	(193	14)
(203	25)	(205	78)	(206	17)	(213	14)	(215	4)
(217	257)	(218	59)	(219	28)	(220	13)	(221	29)
(222	11)	(228	8)	(229	7)	(243	27)	(245	5)
(246	4)	(256	6)	(257	7)	(260	6)	(263	8)
(275	8)	(276	5)	(277	11)	(281	4)	(284	5)
(291	5)	(294	3)	(297	6)	(298	7)	(303	17)
(304	5)	(305	5)	(307	35)	(308	12)	(313	10)
(316	7)	(317	9)	(318	4)	(319	32)	(320	13)
(321	9)	(322	3)	(324	4)	(325	4)	(332	5)
(333	4)	(334	7)	(335	6)	(336	4)	(338	4)
(339	3)	(340	5)	(341	8)	(342	7)	(344	6)
(353	6)	(360	6)	(365	4)	(366	7)	(367	8)
(375	5)	(377	4)	(378	4)	(380	4)	(387	5)
(404	4)	(420	6)	(426	4)	(432	4)	(438	6)
(442	4)	(443	4)	(447	6)	(453	4)	(461	3)
(463	6)	(469	8)	(474	4)	(477	7)	(489	4)
(492	5)	(511	5)	(520	3)	(538	3)	(539	5)
(544	3)	(547	4)	(566	3)				

NAME:12C\_1682.1\_1160EC15\_Aspargine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:168001-10-1

RI:1682

RT:10.676

NUM PEAKS: 96

( 70	21)	( 71	6)	( 72	41)	( 73	1000)	( 74	132)
( 75	279)	( 76	21)	( 77	24)	( 78	3)	( 79	6)
( 84	10)	( 85	6)	( 86	15)	( 87	7)	( 88	4)
( 89	9)	( 90	8)	( 91	3)	( 98	13)	( 99	7)
(100	120)	(101	15)	(102	15)	(103	48)	(104	5)

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(105	5)	(113	4)	(114	26)	(115	33)	(116	427)
(117	60)	(118	23)	(119	6)	(125	10)	(126	3)
(127	3)	(128	21)	(129	10)	(130	34)	(131	75)
(132	209)	(133	65)	(134	15)	(135	5)	(140	3)
(141	119)	(142	23)	(143	13)	(144	16)	(145	4)
(146	8)	(147	161)	(148	28)	(149	25)	(150	3)
(156	3)	(158	6)	(159	48)	(160	10)	(161	4)
(163	3)	(169	8)	(172	12)	(173	4)	(174	9)
(188	122)	(189	27)	(190	18)	(191	4)	(199	4)
(202	36)	(203	9)	(204	14)	(205	5)	(206	3)
(213	3)	(214	3)	(215	17)	(216	11)	(217	20)
(218	37)	(219	8)	(220	4)	(229	3)	(231	147)
(232	33)	(233	14)	(243	8)	(244	4)	(245	3)
(258	25)	(259	7)	(307	5)	(316	4)	(333	7)
(348	7)								

NAME:12C\_1653.8\_1191EC10\_[548; Leucine (2TBS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:165002-10-1

RI:1654

RT:10.407

NUM PEAKS: 176

( 72	23)	( 73	1000)	( 74	85)	( 81	6)	( 82	9)
( 84	5)	( 86	16)	( 87	5)	( 88	3)	( 89	12)
( 90	6)	( 93	12)	( 94	4)	( 97	3)	(100	73)
(101	9)	(102	8)	(103	6)	(105	4)	(107	6)
(109	6)	(110	9)	(112	17)	(114	36)	(115	5)
(121	3)	(122	3)	(125	3)	(126	19)	(128	6)
(130	33)	(131	24)	(132	11)	(133	37)	(135	8)
(137	3)	(138	3)	(140	16)	(141	5)	(142	37)
(143	6)	(144	5)	(146	17)	(147	80)	(148	12)
(149	12)	(150	5)	(152	3)	(153	8)	(154	5)
(155	4)	(157	6)	(158	7)	(159	4)	(160	11)
(161	7)	(163	13)	(164	25)	(165	10)	(167	5)
(170	6)	(171	4)	(172	63)	(173	14)	(174	27)
(178	5)	(179	30)	(181	3)	(185	3)	(186	11)
(187	4)	(188	3)	(193	4)	(194	3)	(198	7)
(199	5)	(200	120)	(201	32)	(202	11)	(203	3)
(211	3)	(213	8)	(214	5)	(215	3)	(216	18)
(217	11)	(218	3)	(220	4)	(225	6)	(227	7)
(236	3)	(241	3)	(243	8)	(245	3)	(249	3)
(252	16)	(253	8)	(254	3)	(268	8)	(270	3)
(271	7)	(272	4)	(281	7)	(285	3)	(289	3)
(296	9)	(298	5)	(301	6)	(302	6)	(305	3)
(310	3)	(311	4)	(313	3)	(314	4)	(315	70)
(316	22)	(317	12)	(321	4)	(329	5)	(330	8)
(331	3)	(337	3)	(338	7)	(342	3)	(345	7)
(346	4)	(347	3)	(354	3)	(357	3)	(359	3)
(364	3)	(365	3)	(366	4)	(367	4)	(371	5)
(376	3)	(377	4)	(378	3)	(382	4)	(386	3)
(390	3)	(391	3)	(393	3)	(394	3)	(407	3)
(409	4)	(412	5)	(417	4)	(418	3)	(419	3)
(424	3)	(435	3)	(436	5)	(440	4)	(441	3)
(448	3)	(453	5)	(462	3)	(463	3)	(480	3)
(483	3)	(484	5)	(495	3)	(498	3)	(499	4)
(507	3)	(511	3)	(513	3)	(522	3)	(533	3)
(543	3)	(545	5)	(546	4)	(549	3)	(557	3)
(563	3)								

NAME:12C\_1509.3\_1178EC16\_[622; Parabanic acid (2TMS)]

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COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:151002-10-1

RI:1509

RT:9.317

NUM PEAKS: 26

( 79	86)	(100	1000)	(101	75)	(102	56)	(115	834)
(116	156)	(128	479)	(131	79)	(144	20)	(153	13)
(158	66)	(171	52)	(201	43)	(202	15)	(207	39)
(243	342)	(244	68)	(245	30)	(257	6)	(261	12)
(431	6)	(457	4)	(518	9)	(523	10)	(544	7)
(568	7)								

NAME:12C\_1481.5\_1160EC15\_[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:148002-10-1

RI:1482

RT:9.067

NUM PEAKS: 16

( 72	9)	( 73	424)	( 74	52)	( 76	48)	( 82	21)
( 84	43)	(100	70)	(112	5)	(139	175)	(147	54)
(148	11)	(155	1000)	(156	183)	(229	28)	(372	15)
(526	18)								

NAME:12C\_1467.9\_1178EC16\_[709; 2,5-Diaminovalerolactam (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:147003-10-1

RI:1468

RT:8.883

NUM PEAKS: 105

( 70	239)	( 71	24)	( 72	70)	( 73	1000)	( 74	128)
( 75	164)	( 76	13)	( 77	11)	( 80	13)	( 82	16)
( 83	8)	( 84	33)	( 85	20)	( 86	85)	( 87	21)
( 88	12)	( 89	11)	( 95	12)	( 96	10)	( 97	11)
( 98	35)	( 99	20)	(100	413)	(101	52)	(102	47)
(103	14)	(104	3)	(105	5)	(106	5)	(110	11)
(111	5)	(112	22)	(113	32)	(114	45)	(115	449)
(116	64)	(117	31)	(118	6)	(119	4)	(124	4)
(125	4)	(126	38)	(127	21)	(128	682)	(129	87)
(130	52)	(131	70)	(132	21)	(133	35)	(134	6)
(135	3)	(137	12)	(138	3)	(139	4)	(140	15)
(141	292)	(142	91)	(143	23)	(144	20)	(145	3)
(146	12)	(147	200)	(148	33)	(149	16)	(152	6)
(153	56)	(154	35)	(155	18)	(156	15)	(157	5)
(158	16)	(159	4)	(160	4)	(167	5)	(168	11)
(169	145)	(170	26)	(171	22)	(172	11)	(173	3)
(174	71)	(175	13)	(176	5)	(185	4)	(186	5)
(187	4)	(188	8)	(200	4)	(203	20)	(204	4)
(214	3)	(215	12)	(216	26)	(217	6)	(227	4)
(229	8)	(230	3)	(241	6)	(242	3)	(243	199)
(244	43)	(245	17)	(257	4)	(258	20)	(259	5)

NAME:12C\_1474.4\_1191EC10\_[NA]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:147002-10-1

RI:1474

RT:8.933

NUM PEAKS: 136

( 70	1000)	( 71	77)	( 72	122)	( 74	33)	( 75	427)
( 76	48)	( 77	13)	( 78	14)	( 79	3)	( 82	5)

160

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( 84 123) ( 86 74) ( 87 13) ( 88 11) ( 89 3)
( 90 51) ( 91 6) ( 92 4) ( 94 4) ( 95 3)
( 97 18) ( 98 68) (100 79) (101 40) (102 14)
(103 11) (104 7) (105 6) (106 4) (107 3)
(111 5) (114 17) (115 31) (116 14) (117 27)
(118 6) (119 4) (122 3) (129 9) (130 28)
(131 27) (132 25) (133 61) (134 14) (135 10)
(136 3) (140 4) (142 100) (143 24) (144 11)
(146 7) (147 14) (148 17) (149 17) (150 6)
(151 4) (153 3) (157 7) (158 12) (159 34)
(160 16) (161 4) (163 3) (164 3) (167 4)
(168 3) (169 3) (170 5) (171 21) (172 8)
(173 5) (174 23) (175 8) (176 6) (184 3)
(185 9) (186 7) (188 7) (190 5) (197 3)
(200 3) (203 4) (204 6) (211 6) (212 3)
(213 3) (216 4) (217 7) (218 65) (219 16)
(220 8) (230 4) (236 7) (240 3) (241 7)
(242 3) (248 8) (256 6) (259 7) (260 5)
(261 4) (273 3) (275 3) (276 12) (277 5)
(292 10) (293 7) (294 4) (305 3) (307 3)
(319 3) (320 15) (321 6) (322 4) (336 3)
(353 4) (354 4) (362 3) (372 3) (376 3)
(407 3) (408 3) (421 3) (422 3) (428 3)
(429 3) (430 3) (435 3) (436 3) (444 3)
(464 3) (465 3) (478 3) (483 3) (490 3)
(494 3)

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NAME:12C\_1296.5\_1191EC10\_Phosphoric acid (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:129001-10-1

RI:1297

RT:6.913

NUM PEAKS: 89

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( 70 7) ( 71 11) ( 72 26) ( 73 1000) ( 74 106)
( 75 97) ( 76 5) ( 77 37) ( 79 6) ( 84 3)
( 85 7) ( 87 12) ( 88 4) ( 89 19) ( 91 10)
(102 5) (103 83) (104 13) (105 28) (106 4)
(107 15) (109 5) (113 3) (115 53) (116 11)
(119 39) (120 6) (121 22) (122 3) (123 10)
(131 36) (132 8) (133 250) (134 34) (135 68)
(136 8) (137 35) (138 4) (139 3) (145 4)
(150 4) (151 23) (152 3) (153 5) (163 8)
(165 13) (166 4) (167 13) (176 3) (177 11)
(178 4) (179 9) (180 3) (181 36) (182 6)
(183 13) (184 3) (189 13) (190 4) (191 50)
(192 12) (193 53) (194 10) (195 14) (196 3)
(197 4) (207 54) (208 11) (209 9) (210 3)
(211 128) (212 19) (213 10) (221 5) (225 24)
(226 5) (227 7) (269 4) (283 24) (284 9)
(285 4) (298 8) (299 436) (300 112) (301 58)
(302 10) (314 62) (315 16) (316 8)

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NAME:12C\_1220.2\_1274EC17\_Valine (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:122001-10-1

RI:1220

RT:6.122

NUM PEAKS: 55

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( 70 15) ( 71 6) ( 72 60) ( 73 846) ( 74 82)
( 75 98) ( 76 7) ( 77 4) ( 82 6) ( 83 4)

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161

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( 84  4) ( 85  5) ( 86 13) ( 87  5) ( 98  4)
( 99  4) (100 114) (101 16) (102  9) (103 24)
(104  3) (105  3) (112  4) (114  9) (115  7)
(116  3) (117 11) (118  3) (119  3) (128 19)
(129 12) (130 12) (131 15) (132 17) (133 26)
(134  4) (142  6) (143  5) (144 1000) (145 134)
(146 49) (147 153) (148 24) (149 14) (156 22)
(157  4) (158  3) (160  3) (163  4) (174  4)
(203  3) (218 143) (219 34) (220 13) (246  9)
```

NAME:12C\_1282.1\_1274EC17\_Serine (2TMS)  
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
 CASNO:128001-10-1  
 RI:1282

RT:6.820

NUM PEAKS: 62

```
( 70 19) ( 71  6) ( 72 25) ( 73 961) ( 74 123)
( 75 316) ( 76 31) ( 81 15) ( 84  3) ( 85  6)
( 86 71) ( 87 24) ( 88 36) ( 89 16) ( 90  6)
( 91 10) ( 96  4) ( 98  4) ( 99  5) (100 110)
(101 24) (102 29) (103 134) (104 14) (105  7)
(114  8) (115  9) (116 1000) (117 112) (118 43)
(119  6) (128  3) (130 71) (131 37) (132 761)
(133 118) (134 35) (142  3) (143  4) (144 134)
(145 16) (146 76) (147 99) (148 19) (149 15)
(159 57) (160  8) (161  4) (172  3) (188 17)
(189  5) (190  4) (206  5) (216  5) (217  4)
(219 33) (220  7) (221  3) (234 31) (235  7)
(236  3) (262  3)
```

NAME:12C\_1326.5\_1274EC17\_Glycine (3TMS)  
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
 CASNO:133001-10-1  
 RI:1327

RT:7.320

NUM PEAKS: 48

```
( 71  4) ( 72 14) ( 73 561) ( 74 44) ( 85  4)
( 86 340) ( 87 29) ( 88 13) ( 99  3) (100 189)
(101 30) (102 23) (103 10) (105  3) (113  5)
(115  4) (116  7) (119  8) (131 21) (133 99)
(134 14) (135  7) (144  6) (147 290) (148 46)
(149 23) (158  7) (159  3) (160 21) (161  4)
(172 10) (173  3) (174 1000) (175 189) (176 83)
(177 18) (188  8) (202  3) (204  4) (246 11)
(247  4) (248 139) (249 42) (250 19) (251  3)
(276 52) (277 14) (278  7)
```

NAME:12C\_1352.5\_1274EC17\_Glyceric acid (3TMS)  
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
 CASNO:135003-10-1  
 RI:1353

RT:7.614

NUM PEAKS: 78

```
( 70 47) ( 71 197) ( 72 20) ( 73 1000) ( 74 74)
( 82 11) ( 83 10) ( 84 28) ( 85 99) ( 89  9)
( 97  3) ( 99 22) (101 28) (102 169) (103 170)
(104 20) (105  8) (106  4) (109  5) (111  6)
(113 21) (115 12) (116 11) (117 88) (118  6)
(119 11) (124  4) (125  3) (126 10) (127 16)
(130 66) (131 35) (133 169) (141  3) (145  4)
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162

(147 458) (148 54) (149 23) (152 3) (155 7)  
(162 4) (163 7) (168 5) (169 13) (173 4)  
(175 9) (177 8) (179 3) (188 3) (189 311)  
(190 50) (191 27) (196 7) (204 10) (205 64)  
(206 9) (207 7) (212 6) (216 4) (217 16)  
(221 30) (222 10) (226 14) (236 4) (241 4)  
(249 3) (251 3) (256 7) (267 18) (268 8)  
(278 4) (281 10) (292 100) (293 31) (294 10)  
(297 3) (306 3) (307 25)

NAME:12C\_1394.9\_1274EC17\_[644; 2-Methyl-1,3-butanediol (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:140003-10-1

RI:1395

RT:8.092

NUM PEAKS: 50

( 71 81) ( 72 29) ( 73 1000) ( 74 85) ( 75 259)  
( 76 23) (101 43) (102 7) (115 29) (116 193)  
(117 836) (118 85) (119 39) (129 20) (130 5)  
(131 33) (133 123) (134 25) (143 175) (144 47)  
(145 33) (147 405) (148 67) (149 140) (150 15)  
(163 9) (175 16) (176 6) (189 5) (203 31)  
(204 7) (217 21) (221 15) (233 62) (234 98)  
(235 25) (236 8) (245 30) (246 9) (291 6)  
(293 4) (299 5) (305 6) (306 107) (307 36)  
(308 18) (309 5) (335 11) (389 4) (405 5)

NAME:12C\_1403.1\_1274EC17\_Threonine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:140001-10-1

RI:1403

RT:8.183

NUM PEAKS: 98

( 71 5) ( 72 23) ( 73 1000) ( 74 93) ( 75 109)  
( 76 8) ( 84 10) ( 85 7) ( 86 19) ( 87 19)  
( 88 6) ( 89 15) ( 98 5) ( 99 5) (100 93)  
(101 187) (102 29) (104 4) (105 8) (106 2)  
(112 4) (113 3) (114 22) (115 22) (116 9)  
(117 303) (118 34) (119 27) (120 3) (128 70)  
(129 88) (130 53) (131 50) (132 46) (133 71)  
(134 17) (135 22) (142 3) (144 6) (145 4)  
(146 13) (147 176) (148 31) (149 21) (150 4)  
(156 3) (158 7) (159 9) (160 9) (161 3)  
(163 8) (165 3) (172 6) (174 6) (175 3)  
(176 4) (177 7) (178 3) (186 5) (188 4)  
(189 5) (190 4) (191 18) (192 13) (193 14)  
(202 25) (203 28) (204 12) (206 5) (207 23)  
(208 12) (209 5) (212 2) (216 4) (217 3)  
(218 211) (219 239) (220 57) (224 20) (226 4)  
(230 7) (231 3) (240 8) (244 2) (248 2)  
(269 4) (282 14) (283 6) (284 3) (291 56)  
(292 35) (293 14) (294 5) (316 2) (320 10)  
(321 5) (329 5) (344 5)

NAME:12C\_1414.0\_1274EC17\_[590; 1-Acetyl-2-thiohydantoin]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:141004-10-1

RI:1414

RT:8.306

NUM PEAKS: 71



163

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( 70 11) ( 72 79) ( 73 774) ( 74 215) ( 75 1000)
( 76 99) ( 77 76) ( 78 6) ( 79 12) ( 80 3)
( 82 9) ( 83 53) ( 84 39) ( 85 11) ( 86 28)
( 87 37) ( 88 13) ( 89 17) ( 90 4) ( 91 19)
( 92 3) ( 93 14) ( 95 5) ( 98 40) ( 99 10)
(100 29) (101 107) (102 29) (103 72) (104 8)
(105 30) (106 3) (112 16) (113 10) (114 117)
(115 20) (116 756) (117 246) (118 30) (119 11)
(126 4) (128 17) (129 50) (130 521) (131 67)
(132 24) (140 24) (141 4) (142 8) (143 10)
(144 23) (145 7) (146 104) (148 73) (149 9)
(150 3) (156 29) (157 12) (158 278) (159 35)
(160 14) (172 7) (173 37) (174 9) (176 22)
(190 7) (191 3) (200 13) (215 4) (218 6)
(233 3)
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NAME:12C\_1440.3\_1274EC17\_[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:144003-10-1

RI:1440

RT:8.603

NUM PEAKS: 63

```
( 70 58) ( 71 6) ( 72 32) ( 73 1000) ( 74 117)
( 75 312) ( 76 30) ( 77 16) ( 84 4) ( 85 4)
( 86 10) ( 87 8) ( 88 6) ( 89 8) ( 91 5)
( 98 6) ( 99 7) (100 53) (101 11) (102 21)
(103 13) (115 7) (116 223) (117 264) (118 36)
(119 12) (128 17) (129 7) (130 310) (131 48)
(132 20) (133 24) (134 4) (135 3) (143 3)
(144 43) (145 6) (146 27) (147 133) (148 24)
(149 18) (150 3) (159 25) (160 581) (161 73)
(162 26) (172 10) (174 6) (187 7) (190 3)
(202 21) (203 4) (220 16) (221 3) (234 33)
(235 8) (236 3) (244 7) (245 50) (246 11)
(247 4) (262 17) (263 3)
```

NAME:12C\_1488.2\_1274EC17\_Malic acid (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:149001-10-1

RI:1488

RT:9.143

NUM PEAKS: 79

```
( 70 7) ( 72 30) ( 73 1000) ( 74 84) ( 75 146)
( 76 13) ( 77 12) ( 78 3) ( 82 5) ( 83 3)
( 84 47) ( 87 6) ( 93 5) ( 99 6) (101 77)
(102 8) (103 13) (105 5) (111 3) (115 10)
(116 12) (117 53) (118 6) (119 9) (129 10)
(131 35) (132 6) (133 126) (134 17) (135 12)
(143 21) (144 5) (145 5) (146 3) (147 505)
(148 76) (149 48) (150 4) (151 6) (171 24)
(172 4) (173 4) (175 48) (176 8) (177 13)
(185 3) (189 63) (190 48) (191 40) (192 9)
(193 3) (203 5) (205 3) (217 25) (218 6)
(219 3) (221 12) (222 3) (233 112) (234 22)
(235 8) (245 66) (246 12) (247 8) (260 3)
(263 14) (264 4) (265 20) (266 4) (305 4)
(306 7) (307 21) (308 9) (309 4) (319 5)
(320 3) (335 26) (336 6) (337 4)
```

NAME:12C\_1565.1\_1274EC17\_Phenylalanine (1TMS)

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COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:157001-10-1

RI:1565

RT:9.777

NUM PEAKS: 49

( 72	4)	( 73	277)	( 74	82)	( 75	218)	( 76	24)
( 77	75)	( 78	12)	( 79	3)	( 80	3)	( 86	17)
( 87	14)	( 88	4)	( 89	14)	( 90	8)	( 91	163)
( 92	29)	( 93	28)	( 94	3)	(100	6)	(102	15)
(103	105)	(104	17)	(105	4)	(116	3)	(117	10)
(118	42)	(119	26)	(120	1000)	(121	96)	(122	3)
(130	233)	(131	38)	(132	9)	(146	460)	(147	48)
(148	19)	(149	3)	(160	3)	(161	3)	(176	11)
(177	14)	(178	3)	(194	10)	(204	37)	(205	11)
(206	3)	(222	30)	(223	5)	(237	3)		

NAME:12C\_1573.9\_1274EC17\_[708; 2,3-Dimethylsuccinic acid (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:157002-10-1

RI:1574

RT:9.844

NUM PEAKS: 85

( 70	9)	( 71	25)	( 72	20)	( 73	1000)	( 74	85)
( 75	205)	( 76	13)	( 77	7)	( 81	5)	( 83	21)
( 85	16)	( 87	3)	( 89	9)	( 95	9)	( 97	45)
( 98	7)	( 99	17)	(101	7)	(102	3)	(103	14)
(110	3)	(111	6)	(113	9)	(115	5)	(117	49)
(119	4)	(127	5)	(131	22)	(132	3)	(133	81)
(134	12)	(135	9)	(141	5)	(143	141)	(144	17)
(145	9)	(147	442)	(148	69)	(149	88)	(150	10)
(151	4)	(157	71)	(158	11)	(161	8)	(169	5)
(171	9)	(177	11)	(184	3)	(185	5)	(189	3)
(190	5)	(191	156)	(192	27)	(193	12)	(213	16)
(217	21)	(218	3)	(220	5)	(221	15)	(222	3)
(231	47)	(232	11)	(233	7)	(243	18)	(244	3)
(245	5)	(259	4)	(265	38)	(266	10)	(267	3)
(275	128)	(276	30)	(277	11)	(287	15)	(288	3)
(289	3)	(299	3)	(305	16)	(306	6)	(307	3)
(349	5)	(350	3)	(377	20)	(378	8)	(379	3)

NAME:12C\_1581.5\_1274EC17\_[680; 2,3-Dimethylsuccinic acid (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:158003-10-1

RI:1582

RT:9.903

NUM PEAKS: 109

( 70	11)	( 71	120)	( 72	29)	( 73	1000)	( 74	88)
( 75	251)	( 76	17)	( 77	11)	( 81	5)	( 83	4)
( 85	8)	( 87	6)	( 89	4)	( 91	37)	( 92	4)
( 93	3)	( 95	21)	( 96	4)	( 97	24)	( 99	11)
(101	7)	(102	3)	(103	12)	(105	4)	(113	61)
(114	5)	(115	66)	(116	10)	(117	70)	(118	7)
(119	9)	(123	11)	(127	5)	(129	38)	(130	5)
(131	40)	(132	7)	(133	80)	(134	11)	(135	9)
(141	14)	(142	3)	(143	43)	(144	7)	(145	6)
(147	493)	(148	78)	(149	95)	(150	13)	(151	6)
(157	108)	(158	18)	(159	8)	(161	3)	(163	20)
(164	3)	(169	18)	(170	3)	(171	10)	(173	4)
(175	4)	(177	3)	(185	50)	(186	9)	(187	5)
(189	12)	(190	6)	(191	10)	(197	4)	(203	5)

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(204	5)	(205	4)	(207	4)	(212	4)	(213	49)
(214	8)	(215	5)	(217	37)	(218	8)	(219	6)
(221	20)	(222	5)	(223	3)	(231	62)	(232	19)
(233	10)	(243	6)	(245	6)	(259	62)	(260	16)
(261	28)	(262	6)	(275	233)	(276	57)	(277	26)
(278	4)	(287	47)	(288	11)	(289	6)	(305	11)
(306	4)	(307	4)	(333	3)	(349	36)	(350	16)
(351	8)	(377	37)	(378	13)	(379	6)		

NAME:12C\_1595.8\_1274EC17\_[639; Proline (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:159001-10-1

RI:1596

RT:10.013

NUM PEAKS: 51

( 70	29)	( 72	85)	( 73	1000)	( 74	92)	( 75	92)
( 78	5)	( 86	12)	( 87	5)	( 89	3)	( 96	6)
( 98	8)	( 99	26)	(100	19)	(101	9)	(102	6)
(105	8)	(106	3)	(107	4)	(113	6)	(115	6)
(116	5)	(119	3)	(126	7)	(129	6)	(131	19)
(132	3)	(133	37)	(134	4)	(140	8)	(142	829)
(143	112)	(144	32)	(147	203)	(148	30)	(149	13)
(170	15)	(171	4)	(172	6)	(186	681)	(187	95)
(188	27)	(193	4)	(216	126)	(217	34)	(218	11)
(244	9)	(288	65)	(289	15)	(290	6)	(303	10)
(304	3)								

NAME:12C\_1625.9\_1274EC17\_Glutamic acid (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:163001-10-1

RI:1626

RT:10.245

NUM PEAKS: 104

( 70	9)	( 71	5)	( 72	36)	( 73	1000)	( 74	108)
( 75	342)	( 76	18)	( 77	8)	( 82	7)	( 83	9)
( 84	343)	( 85	26)	( 86	12)	( 87	8)	( 88	3)
( 89	5)	( 95	6)	( 96	3)	( 98	10)	( 99	4)
(100	97)	(101	19)	(102	10)	(103	11)	(112	13)
(113	11)	(114	22)	(115	21)	(116	4)	(117	23)
(118	3)	(119	7)	(126	3)	(128	392)	(129	67)
(130	31)	(131	31)	(132	23)	(133	68)	(134	10)
(140	45)	(141	7)	(142	6)	(143	6)	(144	6)
(145	5)	(146	7)	(147	263)	(148	44)	(151	3)
(154	4)	(155	4)	(156	255)	(157	45)	(158	61)
(159	3)	(160	5)	(163	4)	(172	5)	(173	6)
(174	57)	(175	7)	(186	11)	(188	4)	(189	5)
(191	3)	(198	3)	(201	3)	(202	8)	(203	6)
(204	33)	(205	7)	(206	4)	(214	10)	(215	4)
(216	6)	(218	35)	(219	10)	(220	4)	(221	12)
(229	3)	(230	117)	(231	28)	(232	13)	(245	11)
(246	695)	(247	149)	(248	63)	(249	8)	(258	19)
(259	5)	(260	3)	(273	3)	(274	6)	(276	5)
(299	4)	(320	6)	(321	3)	(348	32)	(349	10)
(350	5)	(363	15)	(364	6)	(365	3)		

NAME:12C\_1770.3\_1274EC17\_[NA]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:177003-10-1

RI:1770

RT:11.356

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NUM PEAKS: 52

( 82	47)	( 84	40)	( 86	615)	(100	394)	(112	34)
(125	11)	(126	8)	(128	12)	(140	40)	(141	4)
(144	60)	(156	194)	(157	32)	(158	136)	(160	21)
(169	5)	(170	4)	(171	5)	(172	796)	(173	278)
(174	1000)	(175	157)	(176	61)	(185	40)	(187	27)
(199	262)	(200	86)	(201	27)	(202	12)	(214	38)
(215	10)	(217	14)	(230	9)	(231	5)	(239	41)
(244	157)	(245	27)	(246	50)	(247	3)	(273	21)
(274	6)	(305	4)	(329	87)	(330	206)	(331	89)
(332	34)	(345	165)	(346	64)	(347	22)	(361	16)
(362	13)	(363	5)						

NAME:12C\_1794.4\_1274EC17\_[789; Tyramine (3TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:179002-10-1

RI:1794

RT:11.541

NUM PEAKS: 53

( 72	9)	( 73	612)	( 74	57)	( 75	158)	( 76	8)
( 86	350)	( 87	23)	( 88	4)	( 89	93)	( 90	4)
(100	127)	(101	19)	(102	38)	(105	4)	(117	19)
(118	5)	(128	6)	(129	39)	(130	48)	(131	9)
(144	6)	(146	27)	(147	4)	(148	6)	(156	12)
(160	29)	(161	4)	(167	7)	(174	1000)	(175	185)
(176	78)	(183	6)	(190	70)	(191	7)	(199	10)
(217	3)	(223	14)	(230	3)	(231	7)	(238	4)
(239	3)	(244	3)	(246	7)	(255	5)	(260	3)
(287	4)	(331	4)	(345	80)	(346	30)	(347	10)
(348	3)	(361	16)	(362	6)				

NAME:12C\_1806.4\_1274EC17\_[944; D-Mannopyranose (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:181005-10-1

RI:1806

RT:11.634

NUM PEAKS: 148

( 70	12)	( 72	7)	( 73	1000)	( 74	88)	( 75	73)
( 81	23)	( 83	24)	( 87	9)	( 89	28)	( 93	10)
( 94	5)	( 95	4)	( 96	7)	( 97	26)	( 98	5)
(103	56)	(105	10)	(106	8)	(108	4)	(109	5)
(110	3)	(111	15)	(112	3)	(116	3)	(117	81)
(118	6)	(120	4)	(123	4)	(125	13)	(129	109)
(130	20)	(131	35)	(132	5)	(133	56)	(134	8)
(137	4)	(143	23)	(145	7)	(147	201)	(148	42)
(149	27)	(150	5)	(152	6)	(153	3)	(157	17)
(161	5)	(165	4)	(166	4)	(169	7)	(170	3)
(171	5)	(175	10)	(187	3)	(189	56)	(190	19)
(191	567)	(192	97)	(193	40)	(194	15)	(203	22)
(204	839)	(205	159)	(206	66)	(207	14)	(209	5)
(210	5)	(217	141)	(218	37)	(219	16)	(220	6)
(221	8)	(222	8)	(223	6)	(230	5)	(231	22)
(232	5)	(233	6)	(234	4)	(237	18)	(238	7)
(243	13)	(244	3)	(245	4)	(250	4)	(252	3)
(253	3)	(258	3)	(259	4)	(264	3)	(265	8)
(271	6)	(272	3)	(279	7)	(284	3)	(290	3)
(291	10)	(292	6)	(298	3)	(305	15)	(306	8)
(307	4)	(312	13)	(317	8)	(319	3)	(323	5)
(325	4)	(327	3)	(333	3)	(345	13)	(346	3)
(367	5)	(368	8)	(369	4)	(370	5)	(384	3)

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(393	7)	(394	5)	(397	4)	(398	3)	(403	4)
(404	4)	(413	4)	(423	6)	(426	4)	(434	6)
(435	10)	(437	4)	(438	5)	(439	3)	(458	6)
(463	5)	(473	4)	(474	4)	(475	4)	(479	3)
(485	8)	(489	3)	(490	4)	(493	4)	(498	5)
(519	3)	(526	5)	(527	5)	(541	3)	(549	5)
(553	4)	(560	4)	(570	4)				

NAME:12C\_1868.5\_1274EC17\_[826; beta-[(5-methyl-2-thienyl)methylene]amino]-benzeneacetic acid methyl ester]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:187004-10-1

RI:1869

RT:12.112

NUM PEAKS: 78

( 70	8)	( 71	7)	( 72	14)	( 73	962)	( 74	77)
( 75	59)	( 80	3)	( 81	9)	( 85	5)	( 93	4)
( 95	6)	( 97	3)	( 98	11)	( 99	5)	(101	12)
(115	3)	(116	7)	(118	3)	(119	6)	(124	4)
(125	4)	(126	3)	(131	16)	(133	46)	(135	5)
(138	4)	(139	3)	(140	3)	(141	3)	(147	102)
(148	19)	(149	11)	(151	8)	(153	72)	(154	18)
(155	6)	(165	4)	(166	5)	(167	51)	(168	9)
(169	110)	(170	71)	(171	13)	(179	4)	(181	3)
(183	6)	(184	3)	(195	8)	(197	4)	(198	3)
(204	15)	(210	5)	(211	10)	(212	10)	(213	3)
(225	4)	(226	11)	(227	6)	(239	20)	(240	9)
(241	1000)	(242	248)	(243	96)	(244	13)	(267	13)
(268	4)	(269	4)	(284	4)	(315	6)	(341	3)
(343	3)	(356	6)	(374	3)	(431	18)	(432	9)
(433	4)	(446	5)	(447	3)				

NAME:12C\_1877.4\_1274EC17\_alpha-D-Methylglucopyranoside (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:188006-10-1

RI:1877

RT:12.180

NUM PEAKS: 207

( 70	203)	( 73	1000)	( 74	100)	( 81	19)	( 85	13)
( 87	16)	( 89	35)	( 90	6)	( 98	7)	(100	16)
(101	40)	(107	5)	(109	8)	(113	9)	(116	23)
(117	30)	(118	6)	(119	7)	(124	4)	(125	4)
(131	41)	(133	338)	(134	37)	(135	9)	(136	4)
(143	14)	(144	4)	(146	41)	(152	3)	(155	10)
(159	19)	(163	12)	(164	4)	(166	4)	(177	5)
(183	10)	(184	3)	(185	6)	(189	14)	(190	12)
(191	35)	(192	5)	(193	6)	(197	5)	(203	24)
(204	500)	(206	34)	(207	6)	(208	6)	(209	4)
(213	7)	(215	5)	(217	66)	(218	23)	(219	10)
(222	5)	(227	4)	(228	4)	(231	15)	(233	12)
(234	6)	(236	2)	(237	2)	(239	3)	(243	8)
(244	5)	(245	4)	(247	6)	(250	4)	(251	4)
(253	2)	(255	3)	(256	4)	(261	4)	(265	7)
(266	5)	(270	3)	(271	7)	(272	5)	(273	3)
(274	3)	(280	3)	(286	7)	(287	9)	(288	6)
(289	5)	(290	18)	(291	14)	(293	4)	(295	3)
(296	6)	(297	4)	(298	7)	(299	20)	(303	9)
(305	10)	(306	10)	(313	6)	(314	5)	(315	6)
(317	12)	(318	4)	(324	4)	(325	6)	(327	3)
(332	5)	(333	6)	(334	3)	(335	5)	(336	3)

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(337	6)	(338	3)	(341	4)	(345	4)	(349	4)
(353	4)	(361	7)	(371	3)	(372	2)	(374	3)
(376	3)	(377	6)	(381	3)	(382	3)	(385	2)
(386	7)	(387	4)	(388	5)	(391	5)	(393	4)
(396	4)	(399	4)	(400	3)	(405	3)	(408	3)
(409	4)	(412	3)	(413	3)	(414	6)	(415	5)
(429	3)	(430	4)	(431	3)	(436	4)	(437	9)
(438	8)	(439	4)	(446	4)	(448	4)	(450	2)
(451	5)	(454	3)	(456	3)	(457	4)	(461	2)
(464	5)	(469	6)	(472	4)	(473	5)	(476	4)
(477	3)	(478	3)	(480	4)	(482	6)	(485	3)
(486	5)	(489	5)	(490	5)	(491	4)	(495	5)
(496	5)	(497	4)	(501	7)	(503	6)	(507	5)
(508	3)	(510	4)	(511	6)	(514	6)	(515	5)
(517	5)	(518	3)	(521	6)	(524	4)	(526	3)
(529	7)	(533	4)	(535	3)	(536	3)	(538	4)
(539	5)	(541	4)	(547	6)	(548	3)	(549	3)
(553	3)	(557	4)	(559	3)	(563	4)	(565	2)
(567	2)	(568	2)	(569	2)	(574	2)	(576	2)
(578	2)	(584	2)						

NAME:12C\_1889.9\_1274EC17\_Glucose methoxyamine (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:189002-10-1

RI:1890

RT:12.276

NUM PEAKS: 137

( 70	5)	( 71	6)	( 72	20)	( 73	1000)	( 83	24)
( 86	6)	( 89	55)	( 98	3)	( 99	6)	(100	19)
(101	20)	(102	9)	(103	143)	(104	7)	(105	24)
(110	4)	(111	3)	(112	3)	(113	6)	(114	16)
(115	6)	(117	112)	(126	2)	(127	5)	(128	7)
(129	168)	(131	30)	(133	96)	(134	10)	(140	2)
(141	3)	(142	9)	(143	20)	(144	3)	(145	6)
(147	426)	(148	69)	(154	2)	(155	2)	(156	2)
(157	150)	(158	27)	(159	10)	(160	222)	(161	41)
(162	9)	(168	3)	(169	3)	(170	2)	(171	1)
(172	6)	(173	7)	(174	12)	(184	1)	(185	2)
(186	6)	(187	3)	(188	2)	(189	43)	(190	11)
(196	1)	(198	2)	(200	5)	(201	12)	(202	4)
(203	6)	(205	274)	(206	54)	(207	22)	(214	2)
(215	4)	(216	12)	(217	141)	(218	22)	(221	5)
(222	2)	(228	2)	(229	39)	(230	14)	(231	16)
(232	8)	(233	11)	(234	6)	(235	2)	(240	3)
(241	1)	(242	2)	(243	3)	(244	6)	(245	3)
(246	6)	(247	3)	(248	2)	(254	1)	(255	1)
(256	3)	(257	2)	(259	2)	(260	2)	(261	2)
(262	7)	(263	2)	(268	2)	(269	3)	(270	3)
(271	1)	(272	1)	(274	7)	(275	3)	(276	2)
(277	7)	(278	3)	(279	1)	(291	12)	(300	4)
(302	1)	(305	9)	(306	4)	(307	7)	(318	7)
(319	253)	(320	81)	(321	38)	(322	8)	(323	2)
(330	1)	(332	1)	(333	1)	(343	2)	(344	2)
(364	4)	(365	3)	(366	1)	(374	3)	(375	1)
(376	2)	(464	1)						

NAME:12C\_1909.6\_1274EC17\_Glucose methoxyamine {BP} (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:191001-10-1

RI:1910

RT:12.415

NUM PEAKS: 65

( 72	6)	( 73	1000)	( 74	77)	( 75	66)	( 76	3)
( 89	62)	( 90	3)	( 91	3)	(101	11)	(103	186)
(104	17)	(105	23)	(116	4)	(117	84)	(118	7)
(119	8)	(129	127)	(130	8)	(131	23)	(133	83)
(134	10)	(135	6)	(143	12)	(145	3)	(147	304)
(148	42)	(149	28)	(150	3)	(157	97)	(158	11)
(159	8)	(160	134)	(161	27)	(162	7)	(163	12)
(177	6)	(189	30)	(190	24)	(191	15)	(201	6)
(203	3)	(204	24)	(205	195)	(206	41)	(207	21)
(214	3)	(217	86)	(218	16)	(219	6)	(221	6)
(229	27)	(233	16)	(234	4)	(235	6)	(243	3)
(277	9)	(278	5)	(291	7)	(300	3)	(305	4)
(307	5)	(319	183)	(320	57)	(321	26)	(322	5)

NAME:12C\_1915.4\_1274EC17\_Lysine (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:192003-10-1

RI:1915

RT:12.451

NUM PEAKS: 122

( 70	11)	( 71	10)	( 72	19)	( 73	1000)	( 74	110)
( 75	73)	( 76	5)	( 77	3)	( 82	20)	( 83	5)
( 84	36)	( 85	15)	( 86	123)	( 87	16)	( 88	57)
( 89	6)	( 90	4)	( 94	5)	( 97	3)	( 98	11)
( 99	10)	(100	115)	(101	17)	(102	37)	(103	13)
(104	3)	(110	4)	(112	32)	(113	10)	(114	34)
(115	36)	(116	16)	(117	22)	(118	5)	(119	5)
(124	3)	(126	15)	(127	4)	(128	157)	(129	24)
(130	51)	(131	32)	(132	23)	(133	31)	(134	6)
(135	3)	(138	3)	(139	3)	(140	31)	(141	8)
(142	21)	(143	5)	(144	7)	(145	3)	(146	30)
(147	98)	(148	20)	(149	10)	(150	3)	(151	10)
(152	3)	(154	36)	(155	19)	(156	540)	(157	80)
(158	34)	(159	5)	(160	11)	(161	3)	(162	3)
(166	7)	(167	4)	(168	7)	(170	5)	(172	20)
(173	5)	(174	501)	(175	94)	(176	43)	(177	5)
(179	11)	(184	5)	(186	14)	(187	4)	(188	6)
(189	4)	(191	11)	(200	55)	(201	12)	(202	17)
(203	4)	(204	3)	(212	4)	(213	4)	(214	15)
(215	7)	(216	8)	(218	19)	(219	8)	(220	5)
(228	31)	(229	9)	(230	118)	(231	26)	(232	12)
(240	3)	(244	3)	(255	3)	(258	6)	(272	6)
(273	8)	(274	4)	(317	110)	(318	39)	(319	15)
(320	3)	(329	11)	(330	5)	(419	3)	(434	12)
(435	7)	(436	3)						

NAME:12C\_1938.9\_1274EC17\_Tyrosine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:194002-10-1

RI:1939

RT:12.600

NUM PEAKS: 79

( 70	4)	( 72	18)	( 73	1000)	( 74	94)	( 75	108)
( 76	7)	( 77	9)	( 78	4)	( 79	3)	( 82	4)
( 84	4)	( 86	10)	( 87	8)	( 89	9)	( 90	7)
( 91	17)	(100	198)	(101	26)	(102	12)	(103	15)
(104	4)	(105	10)	(115	9)	(116	4)	(117	14)
(118	8)	(119	9)	(130	22)	(131	30)	(132	26)

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(133	32)	(134	7)	(135	11)	(144	3)	(145	4)
(146	11)	(147	267)	(148	47)	(149	41)	(150	6)
(151	5)	(158	3)	(159	3)	(160	7)	(161	5)
(162	3)	(163	22)	(164	8)	(165	12)	(174	7)
(175	5)	(176	7)	(177	7)	(179	122)	(180	28)
(181	8)	(190	5)	(192	16)	(193	6)	(203	5)
(207	7)	(208	7)	(218	883)	(219	179)	(220	79)
(221	10)	(223	3)	(265	9)	(266	3)	(279	4)
(280	68)	(281	18)	(282	6)	(292	3)	(354	14)
(355	7)	(356	4)	(382	8)	(383	3)		

NAME:12C\_2023.7\_1274EC17\_[680; Glycerol-2-phosphate (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:203004-10-1

RI:2024

RT:13.138

NUM PEAKS: 93

( 70	7)	( 72	22)	( 73	1000)	( 74	84)	( 75	188)
( 76	13)	( 77	20)	( 86	5)	( 88	14)	( 89	11)
( 90	3)	( 95	16)	( 99	11)	(101	15)	(103	22)
(105	7)	(111	10)	(113	15)	(114	4)	(115	13)
(121	5)	(125	4)	(126	5)	(127	11)	(130	8)
(131	16)	(133	86)	(134	11)	(135	23)	(137	12)
(141	9)	(142	10)	(143	11)	(147	254)	(148	39)
(149	32)	(150	5)	(151	6)	(153	10)	(155	11)
(160	7)	(161	5)	(163	3)	(167	9)	(168	11)
(169	138)	(170	24)	(171	22)	(177	3)	(179	9)
(181	11)	(183	8)	(184	27)	(185	9)	(186	3)
(193	10)	(195	12)	(197	3)	(198	4)	(200	5)
(207	14)	(208	5)	(211	102)	(212	19)	(213	9)
(215	9)	(225	13)	(227	34)	(228	7)	(229	4)
(241	7)	(242	3)	(243	203)	(244	46)	(245	23)
(253	7)	(256	3)	(257	7)	(258	115)	(259	32)
(260	13)	(285	4)	(297	58)	(298	14)	(299	107)
(300	31)	(301	16)	(302	4)	(315	93)	(316	25)
(317	11)	(370	4)	(485	5)				

NAME:12C\_2029.2\_1274EC17\_[910; 9-(Z)-Hexadecenoic acid (1TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:203002-10-1

RI:2029

RT:13.173

NUM PEAKS: 136

( 70	37)	( 71	26)	( 72	39)	( 73	715)	( 74	83)
( 75	1000)	( 76	70)	( 77	71)	( 78	12)	( 79	85)
( 80	34)	( 81	177)	( 82	84)	( 83	121)	( 84	171)
( 85	34)	( 86	11)	( 87	6)	( 88	5)	( 89	25)
( 90	3)	( 91	37)	( 92	12)	( 93	53)	( 94	30)
( 95	124)	( 96	197)	( 97	108)	( 98	143)	( 99	33)
(100	3)	(101	10)	(102	6)	(103	3)	(105	33)
(106	7)	(107	26)	(108	18)	(109	64)	(110	74)
(111	48)	(112	29)	(113	7)	(115	6)	(116	60)
(117	697)	(118	68)	(119	52)	(120	8)	(121	30)
(122	12)	(123	52)	(124	32)	(125	16)	(126	6)
(127	7)	(128	5)	(129	533)	(130	66)	(131	109)
(132	124)	(133	44)	(134	26)	(135	19)	(136	9)
(137	39)	(138	33)	(139	13)	(140	4)	(141	14)
(142	6)	(143	36)	(144	7)	(145	211)	(146	28)
(148	11)	(149	6)	(150	4)	(151	24)	(152	70)
(153	13)	(154	4)	(155	29)	(156	9)	(157	16)



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(158	7)	(159	18)	(161	7)	(162	4)	(163	4)
(165	14)	(166	13)	(167	4)	(169	3)	(170	6)
(171	25)	(172	10)	(173	12)	(174	4)	(175	3)
(179	6)	(180	5)	(183	16)	(185	49)	(186	12)
(187	10)	(188	5)	(192	9)	(193	11)	(194	48)
(195	7)	(199	62)	(200	12)	(201	12)	(202	3)
(207	4)	(208	7)	(213	12)	(214	3)	(215	4)
(218	3)	(227	7)	(229	8)	(230	3)	(236	32)
(237	7)	(241	4)	(255	3)	(267	4)	(283	4)
(310	4)	(311	136)	(312	39)	(313	9)	(326	15)
(327	5)								

NAME:12C\_1675.0\_1274EC11\_[877; Pyrophosphoric acid (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:168004-10-1

RI:1675

RT:10.627

NUM PEAKS: 96

( 70	7)	( 71	12)	( 72	46)	( 73	1000)	( 74	92)
( 75	44)	( 83	12)	( 85	8)	( 87	3)	( 89	6)
( 91	4)	( 95	6)	( 97	7)	( 98	3)	( 99	5)
(100	6)	(103	21)	(104	5)	(107	5)	(111	4)
(114	3)	(115	9)	(119	10)	(121	14)	(125	3)
(127	21)	(131	6)	(133	61)	(134	7)	(135	43)
(136	4)	(137	11)	(139	4)	(146	13)	(151	9)
(165	8)	(167	5)	(177	5)	(179	5)	(180	3)
(181	10)	(187	3)	(189	5)	(191	24)	(192	7)
(193	48)	(194	7)	(195	28)	(196	4)	(197	6)
(205	5)	(207	57)	(208	12)	(209	10)	(211	10)
(212	3)	(217	17)	(218	5)	(225	13)	(226	3)
(230	3)	(254	3)	(255	7)	(257	4)	(267	3)
(269	12)	(270	3)	(273	3)	(283	16)	(284	6)
(285	26)	(286	6)	(297	4)	(299	74)	(300	18)
(301	8)	(313	6)	(314	7)	(315	3)	(362	3)
(363	24)	(364	7)	(365	4)	(435	4)	(436	4)
(449	5)	(450	55)	(451	369)	(452	150)	(453	80)
(454	21)	(455	6)	(465	5)	(466	35)	(467	15)
(468	9)								

NAME:12C\_1673.8\_1191EC10\_Homocysteine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:167001-10-1

RI:1674

RT:10.561

NUM PEAKS: 223

( 70	16)	( 72	171)	( 75	990)	( 76	88)	( 77	1000)
( 78	54)	( 79	20)	( 82	133)	( 84	120)	( 88	18)
( 89	233)	( 90	28)	( 91	61)	( 92	38)	( 93	136)
( 94	11)	( 95	104)	( 97	29)	( 98	463)	( 99	39)
(101	48)	(102	26)	(103	326)	(104	38)	(105	44)
(106	5)	(107	10)	(111	21)	(114	105)	(119	83)
(120	9)	(121	19)	(122	13)	(124	16)	(125	15)
(127	136)	(128	510)	(129	16)	(130	63)	(137	15)
(139	17)	(142	13)	(144	40)	(146	159)	(155	29)
(156	89)	(157	39)	(161	5)	(162	23)	(165	19)
(166	4)	(167	8)	(171	49)	(176	6)	(183	14)
(184	22)	(185	22)	(187	33)	(193	22)	(200	14)
(201	4)	(202	21)	(203	14)	(212	21)	(214	5)
(224	6)	(228	4)	(229	18)	(230	19)	(234	191)
(235	42)	(236	18)	(241	5)	(244	12)	(250	10)

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(257	10)	(261	10)	(262	14)	(265	6)	(266	7)
(267	7)	(268	23)	(271	30)	(280	5)	(281	4)
(283	11)	(291	4)	(293	4)	(294	6)	(295	10)
(298	6)	(308	19)	(309	4)	(312	5)	(314	38)
(315	12)	(316	17)	(318	9)	(319	18)	(320	9)
(322	12)	(325	10)	(334	19)	(335	8)	(337	16)
(338	7)	(340	10)	(345	10)	(346	22)	(348	6)
(349	4)	(350	17)	(351	14)	(352	9)	(353	8)
(368	4)	(370	9)	(371	13)	(372	5)	(381	5)
(383	10)	(384	4)	(386	4)	(388	5)	(391	6)
(392	10)	(393	10)	(394	12)	(395	15)	(396	3)
(399	3)	(401	7)	(402	6)	(403	5)	(416	6)
(417	5)	(418	11)	(423	6)	(427	6)	(431	7)
(432	13)	(433	7)	(434	6)	(435	6)	(438	11)
(442	5)	(444	9)	(445	11)	(446	6)	(448	8)
(456	5)	(457	16)	(458	12)	(459	7)	(460	7)
(461	10)	(464	14)	(471	4)	(472	10)	(473	10)
(475	5)	(476	5)	(477	4)	(478	18)	(480	6)
(481	7)	(482	3)	(483	16)	(487	12)	(488	4)
(491	17)	(492	12)	(494	8)	(495	11)	(496	4)
(497	4)	(498	7)	(500	8)	(501	10)	(502	9)
(504	8)	(505	19)	(510	8)	(511	5)	(512	6)
(514	4)	(515	8)	(517	13)	(518	3)	(520	8)
(521	16)	(522	10)	(523	4)	(525	6)	(526	5)
(527	6)	(528	10)	(532	7)	(533	6)	(535	7)
(536	8)	(539	7)	(546	6)	(547	7)	(549	3)
(550	5)	(551	7)	(553	6)	(554	7)	(555	10)
(556	3)	(557	6)	(559	4)	(563	5)	(566	4)
(567	7)	(568	7)	(573	6)	(575	3)	(576	3)
(581	5)	(585	3)	(593	3)				

NAME:12C\_1522.3\_1313EC36\_Methionine (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:152001-10-1

RI:1522

RT:8.924

NUM PEAKS: 108

( 73	999)	( 78	21)	( 79	29)	( 93	23)	(108	5)
(122	4)	(128	997)	(129	132)	(166	10)	(176	1000)
(177	142)	(178	78)	(182	7)	(209	8)	(225	7)
(226	9)	(229	7)	(238	8)	(241	3)	(249	5)
(250	53)	(251	13)	(252	7)	(269	8)	(270	6)
(288	6)	(290	10)	(293	55)	(295	12)	(297	5)
(298	8)	(300	4)	(303	3)	(312	6)	(313	10)
(314	4)	(315	8)	(317	4)	(324	3)	(345	8)
(354	7)	(367	5)	(368	8)	(369	6)	(370	4)
(371	8)	(374	6)	(379	5)	(380	3)	(381	9)
(382	6)	(383	7)	(386	4)	(387	5)	(388	9)
(389	4)	(398	6)	(400	3)	(404	3)	(405	3)
(406	7)	(410	4)	(419	5)	(420	5)	(421	9)
(423	3)	(424	4)	(426	6)	(432	4)	(433	7)
(434	7)	(435	4)	(439	5)	(444	6)	(452	8)
(457	6)	(461	7)	(462	10)	(466	4)	(467	6)
(472	5)	(478	6)	(479	5)	(480	4)	(484	7)
(485	7)	(489	4)	(491	4)	(492	5)	(493	4)
(496	4)	(497	7)	(500	7)	(501	4)	(509	5)
(513	5)	(516	3)	(517	4)	(520	3)	(524	4)
(526	6)	(532	4)	(544	5)	(545	3)	(548	10)
(555	5)	(559	4)	(560	4)				

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NAME:12C\_1560.7\_1191EC08\_Cysteine (3TMS)  
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
CASNO:156002-10-1

RI:1561

RT:9.691

NUM PEAKS: 49

( 72	25)	( 73	1000)	( 74	66)	( 75	68)	( 86	15)
( 89	7)	( 95	3)	( 98	3)	( 99	3)	(100	171)
(101	25)	(102	5)	(105	9)	(114	5)	(115	20)
(116	44)	(117	28)	(129	9)	(131	9)	(132	60)
(133	32)	(134	8)	(138	4)	(144	5)	(147	94)
(148	30)	(149	14)	(155	10)	(158	4)	(159	3)
(163	4)	(174	28)	(203	4)	(204	6)	(205	3)
(212	3)	(218	166)	(219	33)	(220	184)	(221	40)
(222	22)	(232	5)	(243	3)	(246	3)	(247	4)
(257	3)	(294	7)	(295	3)	(322	3)		

NAME:12C\_1281.5\_1313EC36\_Ethanolamine (3TMS)  
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1282 |RI:1282  
CASNO:128002-10-1

RI:1282

RT:6.152

SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp

NUM PEAKS: 25

( 72	19)	( 73	1000)	( 74	79)	( 75	133)	( 86	276)
( 87	20)	( 88	19)	(100	284)	(101	33)	(102	25)
(103	26)	(114	30)	(117	30)	(130	53)	(131	45)
(133	83)	(134	8)	(144	24)	(148	14)	(158	7)
(172	10)	(174	945)	(175	165)	(176	57)	(188	8)

NAME:12C\_1364.2\_1313EC11\_Uracil (2TMS)  
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
CASNO:136001-10-1

RI:1364

RT:7.160

NUM PEAKS: 30

( 72	155)	( 73	836)	( 74	77)	( 86	38)	( 96	27)
( 98	37)	( 99	1000)	(100	270)	(101	91)	(103	22)
(105	25)	(109	39)	(113	231)	(114	21)	(117	37)
(126	260)	(127	37)	(131	109)	(133	50)	(147	605)
(148	91)	(153	26)	(169	32)	(239	24)	(241	624)
(242	130)	(243	43)	(255	318)	(256	270)	(257	64)

NAME:12C\_1372.9\_1313EC75\_Fumaric acid (2TMS)  
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
CASNO:137001-10-1

RI:1373

RT:7.260

NUM PEAKS: 37

( 72	44)	( 73	1000)	( 74	116)	( 75	637)	( 77	32)
( 80	12)	( 82	49)	( 83	207)	( 84	81)	(111	12)
(112	19)	(115	105)	(117	23)	(127	62)	(128	21)
(133	150)	(134	22)	(135	32)	(143	183)	(144	26)
(147	940)	(148	150)	(149	114)	(155	73)	(156	29)
(157	37)	(171	21)	(184	23)	(199	16)	(207	20)
(215	16)	(217	43)	(242	12)	(245	650)	(246	139)
(247	70)	(259	29)						

NAME:12C\_1450.0\_1313EC75\_[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]  
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:144007-10-1

RI:1450

RT:8.1600

NUM PEAKS: 162

( 70	5)	( 71	5)	( 72	37)	( 73	1000)	( 74	118)
( 75	311)	( 76	37)	( 77	19)	( 81	2)	( 83	1)
( 84	3)	( 87	19)	( 89	20)	( 90	2)	( 91	3)
( 92	3)	( 93	1)	( 97	5)	( 98	3)	(100	46)
(101	17)	(102	17)	(103	30)	(104	8)	(105	12)
(110	4)	(114	7)	(115	25)	(116	110)	(117	232)
(118	25)	(119	26)	(120	3)	(122	1)	(123	2)
(125	9)	(128	15)	(129	5)	(130	164)	(131	56)
(132	18)	(133	43)	(134	6)	(135	4)	(136	2)
(137	4)	(143	1)	(144	27)	(146	12)	(147	128)
(148	23)	(149	26)	(150	5)	(151	6)	(154	10)
(157	21)	(158	6)	(159	11)	(160	270)	(161	38)
(162	6)	(163	43)	(164	7)	(165	3)	(169	2)
(170	6)	(172	8)	(174	2)	(175	9)	(177	1)
(180	3)	(185	1)	(187	1)	(188	4)	(189	3)
(200	1)	(201	10)	(202	5)	(204	1)	(205	8)
(207	2)	(211	6)	(212	6)	(215	7)	(217	2)
(220	3)	(221	1)	(228	2)	(232	7)	(234	9)
(236	5)	(245	19)	(246	6)	(247	5)	(248	5)
(253	2)	(254	3)	(256	1)	(257	2)	(260	3)
(262	7)	(264	3)	(277	2)	(278	6)	(287	3)
(288	4)	(290	2)	(300	2)	(301	5)	(302	7)
(308	1)	(319	1)	(320	9)	(321	3)	(322	4)
(335	1)	(336	2)	(353	4)	(354	4)	(369	3)
(376	2)	(387	3)	(404	1)	(407	1)	(410	5)
(411	2)	(415	3)	(421	3)	(422	5)	(427	6)
(430	3)	(435	3)	(438	3)	(441	2)	(449	1)
(464	3)	(467	3)	(469	7)	(470	4)	(474	2)
(477	4)	(484	1)	(487	1)	(494	4)	(500	1)
(501	2)	(503	2)	(510	2)	(511	1)	(516	1)
(517	4)	(519	2)	(520	1)	(522	6)	(524	1)
(533	6)	(536	1)	(540	2)	(541	3)	(543	1)
(552	7)	(564	1)						

NAME:12C\_1503.9\_1313EC75\_Erythritol (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:150002-10-1

RI:1504

RT:8.781

NUM PEAKS: 181

( 73	1000)	( 74	80)	( 75	187)	( 76	14)	( 87	6)
( 88	6)	( 89	68)	( 90	5)	(101	43)	(103	155)
(104	15)	(105	11)	(115	37)	(116	51)	(117	136)
(118	12)	(119	13)	(120	3)	(122	2)	(129	53)
(130	4)	(131	38)	(132	4)	(133	87)	(134	11)
(135	10)	(143	28)	(144	3)	(145	9)	(147	338)
(148	51)	(149	35)	(150	4)	(151	3)	(157	10)
(158	3)	(161	5)	(162	2)	(163	14)	(164	3)
(171	7)	(173	6)	(174	3)	(175	10)	(177	5)
(178	2)	(185	4)	(187	5)	(188	2)	(189	56)
(190	11)	(191	40)	(192	8)	(193	3)	(195	2)
(198	2)	(199	4)	(201	21)	(202	3)	(203	13)
(204	53)	(205	90)	(206	19)	(207	9)	(209	5)
(215	7)	(216	3)	(217	173)	(218	35)	(219	13)
(221	9)	(222	5)	(229	6)	(230	3)	(231	11)
(233	2)	(238	3)	(240	2)	(244	2)	(247	5)

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(248	4)	(249	3)	(251	2)	(259	5)	(260	3)
(263	1)	(264	2)	(265	2)	(266	2)	(274	2)
(275	19)	(276	6)	(277	8)	(278	3)	(279	2)
(280	3)	(281	2)	(285	2)	(286	3)	(287	2)
(288	2)	(289	3)	(290	3)	(291	8)	(292	3)
(293	14)	(294	5)	(305	4)	(306	3)	(307	13)
(308	4)	(311	2)	(312	3)	(316	2)	(319	7)
(320	6)	(321	3)	(322	2)	(325	2)	(326	3)
(327	2)	(328	3)	(334	2)	(335	2)	(336	3)
(337	2)	(342	2)	(347	2)	(349	2)	(353	4)
(361	2)	(372	2)	(373	2)	(374	3)	(376	2)
(382	2)	(391	3)	(400	2)	(409	3)	(415	1)
(419	2)	(420	2)	(424	2)	(428	3)	(429	2)
(433	2)	(435	2)	(440	2)	(442	3)	(447	2)
(454	2)	(455	2)	(456	2)	(457	2)	(458	2)
(459	1)	(462	2)	(463	3)	(476	1)	(478	2)
(482	2)	(484	2)	(492	2)	(493	2)	(495	2)
(501	2)	(506	3)	(507	3)	(516	3)	(522	2)
(523	2)	(529	2)	(532	3)	(537	2)	(539	2)
(540	2)	(544	2)	(552	1)	(564	2)	(571	2)
(575	2)								

NAME:12C\_1694.8\_1313EC75\_[746; Ribonic acid-1,4-lactone (3TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:169001-10-1

RI:1695

RT:10.265

NUM PEAKS: 27

( 73	1000)	( 74	77)	( 75	69)	(101	36)	(102	70)
(117	211)	(130	64)	(133	105)	(139	7)	(143	14)
(147	260)	(148	31)	(149	56)	(153	6)	(189	23)
(191	21)	(203	14)	(215	54)	(217	23)	(231	32)
(246	25)	(248	16)	(259	33)	(349	16)	(355	7)
(413	11)	(564	11)						

NAME:12C\_1670.8\_1313EC75\_Arabinose methoxyamine (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1671 |RI:1671 |RI:1671

CASNO:167002-10-1

RI:1671

RT:10.078

SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp

NUM PEAKS: 142

( 70	8)	( 71	6)	( 72	22)	( 73	1000)	( 74	88)
( 75	83)	( 76	4)	( 82	3)	( 83	3)	( 84	4)
( 85	7)	( 86	6)	( 87	8)	( 88	5)	( 89	56)
( 90	5)	( 96	1)	( 99	6)	(100	27)	(101	23)
(102	10)	(103	397)	(104	37)	(105	31)	(111	2)
(112	2)	(113	5)	(114	8)	(115	9)	(116	8)
(117	43)	(118	4)	(119	8)	(125	1)	(126	2)
(127	3)	(128	4)	(129	52)	(130	11)	(131	35)
(132	5)	(133	68)	(134	8)	(136	1)	(140	2)
(141	1)	(142	5)	(143	14)	(144	3)	(145	7)
(146	1)	(147	200)	(148	31)	(149	21)	(150	2)
(151	1)	(152	1)	(154	1)	(156	1)	(157	3)
(158	5)	(159	3)	(160	40)	(161	10)	(162	2)
(163	8)	(164	1)	(165	1)	(168	9)	(169	2)
(170	4)	(171	1)	(172	6)	(173	5)	(174	7)
(175	6)	(176	1)	(177	3)	(184	1)	(186	1)
(187	1)	(188	1)	(189	44)	(190	15)	(191	16)
(192	3)	(193	1)	(198	3)	(199	1)	(200	2)

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(201	3)	(203	3)	(204	18)	(205	21)	(206	4)
(207	3)	(216	5)	(217	199)	(218	41)	(219	18)
(220	2)	(221	5)	(222	1)	(223	1)	(228	1)
(230	1)	(231	3)	(232	2)	(233	15)	(234	6)
(235	1)	(240	1)	(242	3)	(243	1)	(244	1)
(248	2)	(250	1)	(256	3)	(257	2)	(258	5)
(259	1)	(260	1)	(262	5)	(263	1)	(272	1)
(274	2)	(276	1)	(277	15)	(278	5)	(279	2)
(291	3)	(292	1)	(306	3)	(307	65)	(308	19)
(309	9)	(310	1)	(330	1)	(331	1)	(332	1)
(361	1)	(362	1)						

NAME:12C\_1726.7\_1313EC36\_Fucose methoxyamine (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:173002-10-1

RI:1727

RT:10.513

NUM PEAKS: 58

( 72	15)	( 73	1000)	( 74	73)	( 75	131)	( 83	25)
(101	11)	(103	84)	(104	13)	(105	105)	(106	11)
(115	16)	(117	495)	(118	44)	(119	15)	(131	35)
(133	70)	(147	257)	(148	47)	(149	35)	(157	19)
(158	12)	(174	29)	(176	7)	(187	14)	(190	23)
(191	19)	(203	14)	(204	13)	(205	30)	(209	11)
(211	8)	(217	99)	(218	12)	(231	12)	(242	6)
(245	39)	(246	71)	(247	11)	(255	7)	(263	6)
(267	7)	(268	11)	(276	7)	(299	7)	(318	8)
(319	19)	(320	13)	(321	7)	(378	11)	(380	9)
(407	8)	(410	7)	(437	7)	(444	10)	(493	7)
(504	8)	(519	8)	(555	6)				

NAME:12C\_1784.9\_1313EC75\_[798; Ribonic acid (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:179001-10-1

RI:1785

RT:10.966

NUM PEAKS: 44

( 72	16)	( 73	1000)	( 74	81)	( 75	50)	( 89	17)
(101	13)	(102	19)	(103	207)	(104	18)	(105	8)
(117	50)	(119	6)	(130	17)	(131	26)	(132	6)
(133	76)	(134	8)	(143	28)	(145	4)	(147	282)
(148	38)	(175	5)	(189	38)	(190	7)	(191	16)
(205	33)	(206	6)	(207	7)	(217	134)	(218	24)
(219	16)	(221	15)	(222	5)	(257	7)	(277	15)
(278	6)	(292	128)	(293	38)	(294	16)	(305	19)
(306	7)	(307	18)	(331	7)	(333	15)		

NAME:12C\_1806.2\_1313EC75\_[549; 2-Keto-D-gluconic acid (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:181004-10-1

RI:1806

RT:11.131

NUM PEAKS: 57

( 73	1000)	( 74	98)	( 90	8)	(102	16)	(128	11)
(131	24)	(133	40)	(134	12)	(147	160)	(159	17)
(161	12)	(162	12)	(187	131)	(188	28)	(213	15)
(215	18)	(217	126)	(218	33)	(219	23)	(245	8)
(246	10)	(254	9)	(257	56)	(265	6)	(266	11)
(268	8)	(280	9)	(285	9)	(302	9)	(303	14)
(304	8)	(313	11)	(327	12)	(352	11)	(363	11)

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(365	13)	(369	8)	(399	11)	(400	8)	(401	9)
(410	7)	(437	37)	(441	10)	(475	11)	(488	13)
(494	14)	(498	11)	(499	14)	(510	10)	(522	10)
(528	15)	(536	15)	(555	8)	(563	8)	(573	4)
(593	2)	(599	2)						

NAME:12C\_1842.1\_1313EC75\_[693; 2-Furan-2-hydroxyacetic acid (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:184002-10-1

RI:1842

RT:11.411

NUM PEAKS: 122

( 70	8)	( 71	7)	( 72	21)	( 73	1000)	( 74	90)
( 75	144)	( 76	10)	( 77	12)	( 78	1)	( 79	4)
( 80	12)	( 81	83)	( 82	6)	( 83	7)	( 85	11)
( 87	5)	( 88	4)	( 89	13)	( 92	2)	( 93	11)
( 94	7)	( 95	46)	( 96	11)	( 97	14)	( 98	19)
( 99	11)	(100	5)	(101	41)	(106	2)	(107	8)
(108	2)	(109	4)	(110	3)	(111	4)	(112	11)
(113	3)	(115	6)	(117	96)	(118	7)	(119	15)
(121	5)	(122	1)	(123	6)	(124	4)	(125	12)
(126	7)	(127	8)	(131	23)	(132	5)	(133	65)
(134	10)	(135	7)	(137	5)	(138	23)	(139	13)
(140	7)	(147	191)	(148	28)	(149	19)	(150	2)
(151	7)	(152	4)	(153	49)	(154	49)	(155	19)
(166	23)	(167	55)	(168	11)	(169	860)	(170	497)
(171	86)	(172	14)	(175	5)	(179	8)	(180	1)
(181	5)	(182	8)	(183	4)	(193	2)	(194	10)
(195	23)	(196	3)	(197	2)	(199	2)	(205	18)
(206	3)	(207	2)	(209	1)	(210	10)	(211	3)
(212	3)	(227	2)	(239	10)	(240	3)	(241	28)
(242	43)	(243	14)	(255	5)	(256	2)	(257	2)
(267	1)	(268	2)	(269	17)	(270	6)	(271	4)
(283	3)	(284	26)	(285	4)	(286	2)	(313	1)
(329	12)	(330	4)	(331	2)	(358	2)	(359	13)
(360	3)	(373	1)	(374	20)	(375	7)	(376	4)
(377	1)	(390	1)						

NAME:12C\_1848.6\_1313EC75\_[708; Glucose methoxyamine (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:185003-10-1

RI:1849

RT:11.461

NUM PEAKS: 137

( 70	4)	( 71	6)	( 72	18)	( 73	1000)	( 74	86)
( 75	120)	( 76	7)	( 77	6)	( 82	10)	( 83	4)
( 84	2)	( 85	8)	( 86	4)	( 87	6)	( 88	4)
( 89	83)	( 90	7)	( 91	4)	( 92	1)	( 94	1)
( 99	5)	(100	16)	(101	20)	(102	8)	(103	195)
(104	20)	(105	19)	(106	3)	(111	4)	(112	2)
(113	4)	(114	4)	(115	8)	(117	71)	(118	6)
(119	9)	(120	1)	(126	3)	(127	5)	(129	104)
(130	44)	(131	23)	(133	65)	(134	8)	(135	6)
(141	2)	(142	7)	(143	13)	(144	2)	(145	9)
(146	2)	(147	109)	(148	18)	(149	21)	(150	3)
(151	2)	(152	1)	(157	195)	(158	29)	(159	13)
(160	47)	(161	44)	(162	7)	(163	48)	(164	8)
(165	4)	(168	1)	(172	4)	(174	6)	(175	4)
(176	1)	(177	5)	(178	1)	(180	2)	(182	1)
(186	2)	(187	2)	(188	2)	(189	77)	(190	15)

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(191	14)	(192	2)	(193	1)	(196	1)	(198	1)
(200	1)	(202	1)	(203	7)	(204	11)	(205	49)
(206	10)	(212	1)	(214	5)	(215	3)	(216	3)
(217	47)	(218	16)	(219	15)	(220	3)	(228	2)
(229	11)	(230	5)	(231	9)	(232	4)	(233	10)
(234	2)	(235	7)	(236	1)	(237	1)	(240	1)
(243	4)	(244	50)	(245	13)	(246	7)	(247	30)
(248	7)	(249	3)	(259	3)	(260	1)	(261	1)
(262	1)	(268	1)	(270	2)	(274	1)	(275	1)
(276	1)	(278	1)	(291	1)	(302	2)	(304	2)
(305	1)	(319	27)	(320	9)	(321	4)	(322	1)
(333	1)	(337	1)						

NAME:12C\_2113.2\_1313EC36\_[697; Ribose-5-phosphate methoxyamine (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:211003-10-1

RI:2113

RT:13.210

NUM PEAKS: 16

( 73	1000)	( 74	94)	( 89	45)	(129	96)	(133	74)
(147	155)	(157	20)	(207	19)	(211	57)	(217	123)
(299	117)	(300	41)	(315	157)	(316	50)	(317	31)
(459	18)								

NAME:12C\_2225.2\_1313EC36\_Octadecenoic acid (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:223003-10-1

RI:2225

RT:13.896

NUM PEAKS: 126

( 70	45)	( 71	28)	( 72	42)	( 73	1000)	( 75	767)
( 76	50)	( 77	44)	( 80	13)	( 81	109)	( 82	71)
( 83	95)	( 84	111)	( 85	25)	( 86	17)	( 88	12)
( 89	20)	( 94	22)	( 95	93)	( 96	137)	( 97	82)
( 98	100)	( 99	27)	(100	47)	(101	29)	(102	26)
(107	11)	(108	14)	(109	47)	(110	50)	(111	31)
(112	22)	(113	12)	(114	8)	(116	57)	(117	394)
(118	37)	(119	33)	(121	14)	(122	11)	(123	37)
(124	28)	(125	16)	(126	7)	(128	9)	(129	376)
(130	65)	(131	77)	(132	115)	(137	14)	(138	20)
(139	11)	(143	22)	(144	10)	(145	146)	(146	21)
(149	12)	(151	7)	(152	23)	(153	6)	(155	11)
(158	12)	(159	15)	(162	6)	(166	17)	(170	15)
(171	19)	(172	14)	(173	15)	(180	23)	(183	11)
(184	9)	(185	39)	(186	18)	(187	10)	(188	12)
(190	12)	(199	35)	(200	28)	(208	7)	(210	4)
(214	7)	(218	26)	(220	13)	(222	23)	(235	8)
(240	6)	(248	8)	(264	21)	(268	4)	(272	5)
(274	7)	(275	8)	(283	5)	(303	8)	(309	6)
(337	10)	(338	8)	(339	75)	(340	28)	(354	8)
(362	7)	(363	7)	(378	4)	(385	5)	(407	11)
(412	8)	(413	7)	(446	6)	(449	8)	(454	4)
(456	6)	(459	4)	(471	6)	(472	10)	(475	11)
(480	9)	(486	4)	(487	5)	(513	6)	(520	5)
(521	7)	(527	5)	(550	4)	(568	6)	(586	4)
(588	4)								

NAME:12C\_3270.3\_1313EC36\_Ergosterol (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:327001-10-1



RI:3270

RT:19.000

NUM PEAKS: 189

( 70	153)	( 71	80)	( 72	19)	( 73	1000)	( 74	107)
( 75	502)	( 76	64)	( 77	163)	( 78	39)	( 79	251)
( 80	30)	( 81	452)	( 82	78)	( 83	274)	( 84	26)
( 85	27)	( 86	10)	( 87	18)	( 88	9)	( 89	43)
( 90	11)	( 91	309)	( 92	39)	( 93	193)	( 94	32)
( 95	188)	( 96	24)	( 97	81)	( 98	15)	( 99	12)
(101	30)	(102	19)	(103	43)	(104	19)	(105	224)
(106	27)	(107	133)	(108	21)	(109	130)	(110	16)
(111	33)	(113	10)	(114	4)	(115	190)	(116	50)
(117	140)	(118	44)	(119	323)	(120	38)	(121	55)
(122	8)	(123	47)	(124	9)	(125	88)	(126	18)
(127	57)	(128	242)	(129	373)	(130	87)	(131	429)
(132	69)	(133	92)	(134	14)	(135	42)	(136	8)
(137	28)	(138	5)	(139	17)	(140	6)	(141	222)
(142	142)	(143	453)	(144	272)	(145	294)	(146	57)
(147	74)	(148	11)	(149	27)	(150	9)	(151	22)
(152	55)	(153	88)	(154	60)	(155	217)	(156	88)
(157	392)	(158	128)	(159	234)	(160	41)	(161	19)
(162	5)	(163	21)	(164	11)	(165	89)	(166	43)
(167	80)	(168	64)	(169	224)	(170	80)	(171	165)
(172	41)	(173	43)	(174	9)	(175	10)	(176	6)
(177	8)	(178	26)	(179	40)	(180	24)	(181	85)
(182	60)	(183	169)	(184	53)	(185	129)	(186	31)
(187	18)	(188	4)	(189	9)	(191	11)	(192	7)
(193	22)	(194	25)	(196	51)	(197	165)	(198	57)
(199	111)	(200	23)	(201	22)	(202	7)	(205	10)
(206	5)	(207	13)	(208	8)	(209	58)	(211	228)
(212	60)	(213	83)	(214	16)	(215	7)	(219	7)
(223	39)	(224	19)	(225	49)	(226	53)	(227	43)
(228	9)	(229	5)	(238	29)	(239	55)	(240	14)
(241	6)	(247	3)	(248	3)	(251	68)	(252	33)
(253	164)	(254	37)	(255	6)	(265	21)	(266	7)
(267	13)	(268	4)	(279	12)	(280	12)	(281	8)
(293	13)	(294	6)	(295	4)	(310	5)	(323	5)
(326	10)	(327	6)	(335	6)	(336	17)	(337	227)
(338	82)	(339	18)	(343	6)	(363	317)	(364	119)
(365	21)	(377	14)	(378	79)	(379	31)	(380	5)
(467	9)	(468	53)	(469	28)	(470	8)		

NAME:12C\_1580.7\_1313EC75\_[829; 1-Phenylethanol (1TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:158002-10-1

RI:1581

RT:9.378

NUM PEAKS: 10

( 82	34)	(179	1000)	(180	165)	(181	44)	(193	105)
(194	19)	(267	71)	(268	15)	(269	6)	(284	6)

NAME:12C\_2109.7\_1313EC75\_[662; Ribose-5-phosphate methoxyamine {BP} (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:211004-10-1

RI:2110

RT:13.188

NUM PEAKS: 47

( 72	27)	( 73	1000)	( 74	90)	( 75	151)	( 77	24)
( 89	42)	( 98	13)	(100	40)	(101	45)	(104	8)
(105	22)	(114	12)	(115	15)	(117	75)	(119	14)

180

(129	122)	(130	31)	(131	42)	(132	33)	(133	69)
(135	24)	(138	7)	(143	14)	(145	21)	(147	232)
(158	31)	(160	40)	(175	5)	(189	17)	(191	16)
(195	10)	(207	13)	(211	46)	(212	13)	(217	118)
(218	29)	(219	10)	(225	13)	(299	96)	(300	31)
(301	13)	(315	143)	(316	39)	(321	8)	(357	16)
(387	9)	(403	14)						

NAME:12C\_2125.3\_1313EC75\_[832; Dopamine (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:213003-10-1

RI:2125

RT:13.287

NUM PEAKS: 53

( 72	18)	( 73	816)	( 74	58)	( 75	62)	( 77	7)
( 86	118)	( 89	9)	( 96	5)	(100	38)	(102	20)
(103	20)	(104	14)	(114	9)	(115	9)	(117	58)
(128	12)	(130	23)	(131	27)	(133	29)	(139	7)
(143	13)	(147	282)	(148	40)	(161	8)	(172	13)
(174	1000)	(175	190)	(176	68)	(177	6)	(178	7)
(188	8)	(189	19)	(204	17)	(205	21)	(207	5)
(216	7)	(217	26)	(218	9)	(248	4)	(259	9)
(288	5)	(290	17)	(291	12)	(299	6)	(304	9)
(307	10)	(344	5)	(355	5)	(396	6)	(443	5)
(475	4)	(591	4)	(599	3)				

NAME:12C\_2155.6\_1313EC75\_[795; Erythritol (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:216003-10-1

RI:2156

RT:13.479

NUM PEAKS: 106

( 72	14)	( 73	1000)	( 74	86)	( 80	5)	( 84	7)
( 86	10)	( 88	22)	( 93	3)	( 94	3)	(100	6)
(103	163)	(104	18)	(105	12)	(107	4)	(108	3)
(114	7)	(116	19)	(117	86)	(118	9)	(119	7)
(127	5)	(128	7)	(129	46)	(130	17)	(131	16)
(132	4)	(133	46)	(134	7)	(135	5)	(140	4)
(141	6)	(142	26)	(143	15)	(144	12)	(145	3)
(146	26)	(147	239)	(148	36)	(149	27)	(150	3)
(151	3)	(155	4)	(157	27)	(158	14)	(163	3)
(168	9)	(169	9)	(172	7)	(173	16)	(174	43)
(175	7)	(179	3)	(180	4)	(181	3)	(184	3)
(189	20)	(191	12)	(196	3)	(197	14)	(198	7)
(200	11)	(201	4)	(202	3)	(203	5)	(204	17)
(205	60)	(206	14)	(207	9)	(216	4)	(217	77)
(218	19)	(219	6)	(221	12)	(228	4)	(229	25)
(230	6)	(231	3)	(232	4)	(243	9)	(256	7)
(257	7)	(259	3)	(269	4)	(311	5)	(313	4)
(314	11)	(315	7)	(319	8)	(320	3)	(339	6)
(343	4)	(344	5)	(345	26)	(346	9)	(347	4)
(357	6)	(370	5)	(371	4)	(375	5)	(429	6)
(433	3)	(435	3)	(519	10)	(520	3)	(521	3)
(523	3)								

NAME:12C\_2162.3\_1313EC75\_[648; Ethylamine (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:216002-10-1

RI:2162

RT:13.521

181

NUM PEAKS: 54

( 72	18)	( 73	1000)	( 74	79)	( 75	51)	( 86	127)
( 87	17)	( 89	31)	(100	88)	(101	23)	(102	17)
(103	161)	(104	15)	(106	4)	(115	7)	(117	64)
(118	9)	(129	34)	(130	20)	(132	6)	(133	39)
(134	6)	(143	9)	(157	10)	(172	25)	(173	9)
(174	283)	(175	54)	(176	20)	(185	12)	(189	17)
(190	8)	(199	5)	(200	4)	(204	13)	(205	45)
(206	10)	(207	5)	(216	10)	(217	93)	(218	19)
(219	9)	(231	4)	(241	16)	(259	6)	(267	7)
(272	16)	(287	15)	(288	6)	(305	7)	(306	3)
(307	15)	(314	11)	(315	12)	(346	5)		

NAME:12C\_2168.9\_1313EC75\_[705; 2-Ketogluconic acid (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:217002-10-1

RI:2169

RT:13.563

NUM PEAKS: 52

( 72	21)	( 73	1000)	( 74	81)	( 75	70)	( 79	5)
( 86	63)	( 87	12)	( 89	11)	(100	35)	(102	10)
(103	35)	(115	6)	(116	5)	(117	26)	(129	37)
(130	16)	(131	28)	(133	34)	(134	9)	(141	30)
(142	8)	(145	4)	(147	269)	(148	43)	(149	25)
(150	5)	(156	5)	(157	17)	(167	4)	(170	4)
(172	8)	(174	104)	(175	22)	(176	8)	(189	16)
(191	41)	(192	8)	(205	17)	(207	7)	(215	11)
(217	47)	(218	13)	(257	45)	(258	12)	(303	12)
(304	7)	(319	12)	(425	3)	(436	9)	(437	40)
(438	20)	(439	9)						

NAME:12C\_2180.5\_1313EC75\_[733; Threitol (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:218001-10-1

RI:2181

RT:13.637

NUM PEAKS: 128

( 70	7)	( 72	20)	( 73	1000)	( 74	89)	( 75	131)
( 76	9)	( 77	6)	( 80	8)	( 81	7)	( 82	7)
( 83	25)	( 86	11)	( 87	7)	( 88	6)	( 89	43)
( 94	4)	( 95	14)	( 97	4)	( 98	5)	(100	11)
(101	17)	(102	8)	(103	194)	(104	18)	(105	11)
(107	7)	(109	5)	(114	9)	(115	7)	(116	20)
(117	74)	(119	8)	(125	3)	(127	5)	(128	9)
(129	40)	(130	15)	(131	22)	(132	5)	(133	51)
(134	6)	(139	5)	(140	4)	(142	32)	(144	20)
(145	7)	(146	43)	(147	222)	(148	35)	(149	25)
(150	4)	(152	4)	(155	5)	(156	5)	(157	14)
(158	29)	(159	6)	(160	8)	(163	5)	(167	5)
(168	8)	(169	9)	(172	10)	(173	24)	(174	66)
(175	12)	(176	4)	(181	7)	(183	5)	(185	10)
(186	9)	(187	5)	(188	3)	(189	18)	(190	5)
(191	10)	(195	3)	(197	26)	(198	8)	(199	3)
(200	6)	(202	3)	(203	3)	(205	38)	(206	8)
(207	6)	(215	4)	(216	6)	(217	81)	(218	20)
(219	8)	(221	9)	(223	6)	(229	14)	(230	4)
(232	6)	(243	8)	(253	4)	(255	4)	(256	7)
(268	5)	(270	3)	(271	4)	(277	4)	(287	5)
(291	3)	(295	4)	(307	5)	(313	5)	(314	12)
(315	7)	(339	7)	(340	3)	(343	5)	(344	5)

182

(345 40) (346 12) (347 4) (370 5) (371 3)  
 (375 6) (429 6) (430 3) (433 4) (518 3)  
 (519 8) (523 8) (524 4)

NAME:12C\_2245.5\_1313EC75\_Octadecanoic acid (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:225002-10-1

RI:2246

RT:14.001

NUM PEAKS: 124

( 70 33) ( 71 65) ( 72 50) ( 73 932) ( 74 104)  
 ( 75 1000) ( 76 73) ( 77 57) ( 78 3) ( 79 29)  
 ( 80 4) ( 81 78) ( 82 12) ( 83 87) ( 84 26)  
 ( 85 39) ( 86 13) ( 88 7) ( 89 29) ( 90 5)  
 ( 91 13) ( 92 3) ( 93 27) ( 94 4) ( 95 69)  
 ( 96 12) ( 97 66) ( 98 48) ( 99 28) (100 4)  
 (101 15) (102 6) (105 28) (106 3) (107 14)  
 (109 22) (110 4) (111 32) (112 14) (113 6)  
 (115 10) (116 65) (117 947) (118 94) (119 39)  
 (121 11) (123 7) (125 9) (126 4) (127 6)  
 (128 4) (129 493) (130 64) (131 162) (132 487)  
 (133 105) (134 25) (135 12) (137 3) (139 5)  
 (140 4) (141 5) (143 51) (144 7) (145 282)  
 (146 39) (149 5) (151 3) (153 5) (154 9)  
 (155 7) (157 15) (158 3) (159 33) (160 6)  
 (163 3) (167 4) (168 3) (171 28) (172 4)  
 (173 8) (174 4) (185 44) (186 7) (187 25)  
 (188 9) (199 12) (201 76) (202 13) (203 4)  
 (210 3) (213 10) (214 3) (215 11) (216 3)  
 (223 5) (227 13) (228 3) (229 6) (230 3)  
 (241 13) (242 3) (243 11) (244 3) (255 7)  
 (257 17) (258 4) (269 3) (271 7) (283 3)  
 (285 3) (297 15) (298 6) (299 6) (313 15)  
 (314 5) (340 19) (341 216) (342 68) (343 17)  
 (355 3) (356 37) (357 12) (358 3)

NAME:12C\_2328.1\_1313EC75\_Glucose-6-phosphate methoxyamine (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:233002-10-1

RI:2328

RT:14.440

NUM PEAKS: 123

( 70 4) ( 72 17) ( 73 1000) ( 74 88) ( 75 83)  
 ( 76 4) ( 77 10) ( 82 7) ( 86 6) ( 87 6)  
 ( 88 3) ( 89 34) ( 90 3) ( 99 5) (100 12)  
 (101 38) (102 11) (104 4) (105 24) (106 4)  
 (107 3) (113 6) (114 10) (115 12) (116 16)  
 (119 7) (121 3) (127 4) (129 69) (130 17)  
 (131 27) (132 4) (133 65) (134 9) (135 16)  
 (137 6) (138 3) (141 3) (142 5) (143 11)  
 (145 7) (147 141) (148 22) (149 18) (150 3)  
 (151 7) (156 3) (157 35) (158 9) (159 4)  
 (160 94) (161 19) (162 4) (163 6) (169 4)  
 (173 4) (181 8) (189 11) (190 3) (191 16)  
 (193 10) (195 8) (196 3) (197 3) (204 17)  
 (205 7) (207 16) (208 4) (209 3) (210 4)  
 (211 43) (212 9) (213 5) (215 4) (216 6)  
 (217 36) (218 9) (219 4) (221 3) (225 13)  
 (226 3) (227 9) (228 6) (229 5) (231 7)  
 (243 5) (244 3) (246 3) (253 4) (268 3)

183

(269	5)	(274	3)	(283	4)	(285	5)	(298	10)
(299	104)	(300	30)	(301	14)	(302	3)	(313	3)
(314	7)	(315	41)	(316	12)	(317	6)	(331	13)
(332	4)	(341	6)	(342	3)	(356	6)	(357	37)
(358	12)	(359	6)	(373	3)	(385	3)	(386	30)
(387	122)	(388	47)	(389	25)	(390	7)	(470	4)
(471	12)	(472	6)	(473	3)				

NAME:12C\_2383.7\_1313EC75\_[724; Glycerol (3TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:238002-10-1

RI:2384

RT:14.735

NUM PEAKS: 34

( 72	16)	( 73	1000)	( 74	80)	( 75	108)	( 87	7)
( 89	36)	(103	153)	(104	11)	(116	8)	(117	196)
(118	17)	(129	29)	(130	9)	(131	17)	(133	41)
(142	35)	(143	11)	(144	15)	(147	208)	(148	30)
(149	21)	(158	89)	(159	23)	(160	19)	(171	7)
(173	9)	(183	15)	(189	13)	(201	8)	(205	34)
(216	8)	(217	71)	(218	18)	(276	12)		

NAME:12C\_2564.4\_1313EC75\_[945; Galactofuranose-6-phosphate (7TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:256001-10-1

RI:2564

RT:15.695

NUM PEAKS: 263

( 72	20)	( 73	1000)	( 74	85)	( 75	90)	( 76	14)
( 77	12)	( 79	12)	( 84	17)	( 86	5)	( 87	6)
( 88	8)	( 89	47)	( 90	6)	( 91	7)	( 92	3)
( 96	5)	( 98	3)	(100	9)	(101	31)	(103	102)
(105	16)	(106	9)	(107	6)	(115	12)	(116	18)
(117	28)	(119	11)	(120	5)	(121	7)	(128	7)
(129	76)	(130	17)	(131	34)	(132	8)	(133	80)
(134	15)	(135	19)	(136	3)	(137	10)	(139	3)
(142	10)	(143	10)	(144	9)	(145	9)	(146	6)
(147	160)	(148	24)	(151	5)	(153	5)	(156	8)
(157	35)	(158	10)	(159	8)	(162	7)	(163	12)
(165	3)	(166	3)	(171	4)	(172	13)	(173	17)
(174	8)	(175	8)	(176	4)	(181	9)	(185	5)
(186	6)	(188	7)	(189	14)	(190	5)	(191	17)
(195	8)	(196	6)	(197	3)	(200	7)	(201	7)
(202	8)	(203	10)	(204	16)	(205	14)	(206	6)
(207	15)	(208	6)	(210	5)	(211	34)	(212	5)
(214	7)	(216	7)	(217	50)	(218	14)	(219	4)
(220	6)	(222	5)	(223	3)	(225	15)	(226	8)
(227	10)	(228	7)	(229	5)	(230	5)	(231	6)
(232	6)	(233	6)	(235	6)	(236	4)	(239	3)
(240	4)	(241	4)	(245	5)	(249	7)	(250	4)
(251	6)	(253	4)	(259	6)	(260	5)	(264	4)
(265	6)	(266	4)	(267	8)	(268	4)	(269	9)
(270	7)	(271	4)	(273	6)	(274	6)	(275	5)
(276	6)	(281	5)	(282	5)	(283	10)	(284	8)
(285	8)	(291	3)	(292	5)	(293	4)	(295	3)
(296	5)	(298	10)	(299	92)	(300	25)	(301	17)
(302	4)	(303	3)	(305	7)	(306	5)	(307	8)
(308	4)	(312	3)	(313	7)	(314	5)	(315	38)
(316	15)	(317	9)	(318	5)	(319	5)	(320	4)
(321	6)	(324	4)	(326	4)	(327	5)	(328	5)

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(331	12)	(332	9)	(333	7)	(340	5)	(341	8)
(344	3)	(346	3)	(348	4)	(349	6)	(350	7)
(353	5)	(354	3)	(355	6)	(356	10)	(357	35)
(358	14)	(359	8)	(362	5)	(363	4)	(364	3)
(365	4)	(369	6)	(370	6)	(371	7)	(372	6)
(373	6)	(377	4)	(382	3)	(384	4)	(385	7)
(386	28)	(387	115)	(388	44)	(389	28)	(390	9)
(391	5)	(393	3)	(396	5)	(400	4)	(403	6)
(404	3)	(405	6)	(408	5)	(409	4)	(413	3)
(417	7)	(418	6)	(423	5)	(427	4)	(428	3)
(442	6)	(443	3)	(444	3)	(448	7)	(449	4)
(452	3)	(457	6)	(458	8)	(459	3)	(461	5)
(471	17)	(472	7)	(473	6)	(475	3)	(483	6)
(484	3)	(485	3)	(486	5)	(487	6)	(488	4)
(490	4)	(491	4)	(492	4)	(495	7)	(496	5)
(499	3)	(500	4)	(502	3)	(509	5)	(513	7)
(514	3)	(517	6)	(520	6)	(525	4)	(526	4)
(527	5)	(528	4)	(530	7)	(531	6)	(533	3)
(538	5)	(541	3)	(545	3)	(547	4)	(548	3)
(549	3)	(550	3)	(554	4)	(560	4)	(561	4)
(564	4)	(566	4)	(572	4)				

NAME:12C\_2619.2\_1313EC75\_[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:262001-10-1

RI:2619

RT:15.985

NUM PEAKS: 126

( 70	4)	( 71	6)	( 72	15)	( 73	1000)	( 74	87)
( 75	134)	( 76	8)	( 77	10)	( 81	25)	( 83	5)
( 85	9)	( 87	7)	( 88	3)	( 89	17)	( 91	3)
( 95	3)	( 97	7)	( 99	9)	(101	27)	(102	5)
(103	193)	(104	18)	(105	11)	(109	13)	(111	10)
(113	10)	(115	9)	(116	18)	(117	78)	(118	8)
(119	8)	(127	7)	(129	177)	(130	22)	(131	39)
(132	10)	(133	53)	(134	7)	(135	6)	(139	4)
(141	6)	(142	6)	(143	28)	(144	5)	(145	18)
(146	3)	(147	214)	(148	34)	(149	36)	(150	5)
(151	4)	(153	7)	(155	46)	(156	8)	(157	37)
(158	6)	(159	9)	(161	3)	(163	6)	(169	89)
(170	15)	(171	18)	(172	3)	(173	14)	(175	5)
(177	6)	(183	19)	(184	3)	(185	3)	(189	33)
(190	8)	(191	123)	(192	22)	(193	11)	(199	25)
(200	4)	(201	4)	(203	13)	(204	57)	(205	23)
(206	7)	(207	5)	(215	6)	(216	5)	(217	307)
(218	74)	(219	39)	(220	6)	(221	9)	(227	3)
(229	6)	(230	6)	(231	15)	(232	5)	(233	7)
(234	3)	(241	3)	(242	4)	(243	40)	(244	11)
(245	13)	(246	3)	(247	6)	(257	5)	(259	20)
(260	6)	(263	6)	(271	27)	(272	7)	(273	11)
(274	3)	(289	25)	(290	7)	(291	7)	(305	5)
(319	9)	(320	4)	(331	20)	(332	16)	(333	7)
(360	13)	(361	126)	(362	45)	(363	21)	(364	5)
(377	4)								

NAME:12C\_2656.9\_1313EC75\_[559; Erythritol (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:266001-10-1

RI:2657

RT:16.186

NUM PEAKS: 42

( 70	175)	( 72	21)	( 73	1000)	( 74	83)	( 75	109)
( 80	19)	( 81	16)	( 82	45)	( 83	15)	( 89	44)
( 98	52)	( 99	122)	(100	21)	(103	162)	(113	15)
(116	16)	(117	56)	(125	36)	(127	130)	(128	21)
(129	58)	(131	29)	(133	55)	(147	201)	(148	37)
(149	29)	(155	15)	(156	16)	(169	37)	(170	18)
(171	44)	(185	29)	(189	14)	(196	25)	(217	97)
(218	25)	(238	14)	(267	27)	(268	44)	(292	50)
(298	48)	(323	21)						

NAME:12C\_2733.0\_1313EC75\_[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:273002-10-1

RI:2733

RT:16.590

NUM PEAKS: 78

( 70	3)	( 72	11)	( 73	1000)	( 74	85)	( 82	17)
( 83	4)	( 85	5)	( 86	5)	( 87	4)	( 88	4)
( 89	48)	( 90	3)	(100	7)	(101	19)	(102	5)
(103	113)	(104	9)	(105	32)	(106	3)	(113	5)
(114	6)	(115	5)	(116	8)	(117	77)	(118	9)
(119	5)	(128	4)	(130	10)	(131	14)	(132	3)
(133	44)	(140	3)	(141	4)	(143	15)	(147	303)
(148	48)	(149	26)	(156	4)	(160	85)	(161	20)
(162	5)	(163	5)	(169	37)	(170	7)	(175	3)
(186	10)	(187	3)	(189	23)	(190	3)	(203	6)
(204	267)	(205	112)	(206	33)	(207	11)	(215	4)
(216	6)	(218	17)	(221	5)	(222	3)	(229	7)
(230	3)	(243	19)	(244	35)	(245	12)	(269	5)
(270	3)	(271	18)	(272	4)	(307	6)	(318	4)
(319	23)	(320	9)	(360	20)	(361	169)	(362	60)
(363	26)	(390	3)	(451	4)				

NAME:12C\_2826.4\_1313EC75\_[855; Squalene]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:283001-10-1

RI:2826

RT:17.062

NUM PEAKS: 34

( 70	112)	( 79	130)	( 80	53)	( 81	1000)	( 82	107)
( 87	13)	( 92	36)	( 93	202)	( 95	280)	( 97	45)
(107	124)	(108	40)	(109	123)	(118	14)	(120	20)
(121	171)	(122	37)	(123	102)	(132	9)	(135	89)
(136	134)	(137	123)	(138	11)	(149	107)	(158	24)
(163	31)	(173	24)	(174	16)	(175	26)	(203	30)
(231	33)	(259	18)	(260	15)	(363	10)		

NAME:12C\_2871.8\_1313EC75\_Isomaltose methoxyamine (8TMS); alpha-D-Glc-(1,6)-D-Glc (8TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:287001-10-1

RI:2872

RT:17.263

NUM PEAKS: 126

( 70	5)	( 71	5)	( 72	15)	( 73	1000)	( 74	87)
( 75	96)	( 81	15)	( 82	4)	( 83	4)	( 85	8)
( 86	4)	( 87	7)	( 88	3)	( 89	33)	( 90	3)

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( 97   5) ( 99   8) (100  17) (101  36) (102  12)
(103 125) (104  12) (105  24) (109   7) (111   6)
(113   7) (114   6) (115   9) (116  20) (117  72)
(118   7) (119   6) (127   5) (128   4) (129 122)
(130  20) (131  30) (132   6) (133  56) (134   7)
(135   5) (139   3) (141   5) (142   7) (143  23)
(144   4) (145   9) (147 236) (148  37) (149  28)
(150   3) (151   3) (153   4) (155  18) (156   4)
(158   6) (159   5) (160  95) (161  39) (162   7)
(163   9) (169  67) (170  11) (171   8) (172   3)
(173   6) (174   3) (175   4) (177   4) (183   5)
(189  32) (190   9) (191  52) (192   9) (193   4)
(201   3) (203  14) (204 215) (205  57) (206  20)
(207   7) (215   5) (216   7) (217 135) (218  34)
(219  15) (221   9) (228   5) (229   7) (230   5)
(231  16) (232   5) (233   8) (234   3) (241   3)
(243  31) (244  10) (245   8) (246   5) (247   5)
(257   3) (259   6) (262   3) (271  24) (272   6)
(273   6) (274   4) (275   3) (291   7) (300   3)
(305   8) (306   4) (307   5) (317   3) (318   3)
(319  15) (320   5) (331   6) (332   5) (360  18)
(361 158) (362  56) (363  25) (364   9) (390   4)
(480   4)

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NAME:12C\_2906.7\_1313EC75\_Isomaltose methoxyamine {BP} (8TMS); alpha-D-Glc-(1,6)-D-Glc (8TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:291002-10-1

RI:2907

RT:17.418

NUM PEAKS: 64

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( 72  14) ( 73 1000) ( 74   80) ( 75   86) ( 81  13)
( 87   7) ( 89   41) (100   18) (101  36) (102  11)
(103 166) (104  15) (105  15) (115   7) (117  69)
(118   8) (129 110) (130  17) (131  29) (132   6)
(133  73) (134   9) (143  20) (147 235) (148  37)
(149  28) (155  17) (157  19) (160  77) (161  41)
(163   9) (169  65) (170  11) (171   6) (173   6)
(189  29) (190   8) (191  51) (192   8) (201   5)
(203  15) (204 212) (205  60) (206  19) (216   4)
(217 106) (218  29) (219  13) (221   6) (229   7)
(233  16) (243  29) (244   9) (271  22) (273  12)
(274   4) (305   9) (319  14) (331   6) (332   4)
(360  19) (361 152) (362  56) (363  27)

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NAME:12C\_2811.2\_1160EC39\_[895; Isomaltose methoxyamine (8TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:281001-10-1

RI:2811

RT:17.476

NUM PEAKS: 89

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( 73 1000) ( 74   66) ( 75   95) ( 89   31) (101  47)
(103  92) (104  28) (105  26) (109   8) (116  13)
(117  75) (118   9) (129 104) (131  19) (133  36)
(134   8) (143  19) (147 179) (148  39) (150   9)
(157  13) (160  85) (161  45) (164  17) (169  21)
(171  10) (174  10) (189  24) (191  47) (203  10)
(204 304) (205  63) (206  37) (214  12) (217 102)
(218  34) (219  11) (228  18) (230  12) (240  14)
(243  30) (244   8) (245   5) (248  13) (259  11)

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187

(262	9)	(271	35)	(273	13)	(276	11)	(287	9)
(304	6)	(319	14)	(322	10)	(325	6)	(342	9)
(344	7)	(346	8)	(352	12)	(361	87)	(362	45)
(363	21)	(365	12)	(367	8)	(375	12)	(395	14)
(396	7)	(399	9)	(405	5)	(407	7)	(420	7)
(421	5)	(433	12)	(436	6)	(439	10)	(463	11)
(464	16)	(468	7)	(475	11)	(480	10)	(482	6)
(486	7)	(493	7)	(497	16)	(506	11)	(527	7)
(529	18)	(562	11)	(564	5)	(581	3)		

NAME:12C\_2518.0\_1313EC75\_[644; Erythritol (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:252002-10-1

RI:2518

RT:15.448

NUM PEAKS: 176

( 70	13)	( 71	26)	( 72	19)	( 73	1000)	( 74	84)
( 75	108)	( 76	5)	( 77	6)	( 78	3)	( 79	4)
( 80	8)	( 81	8)	( 82	13)	( 83	15)	( 84	14)
( 85	22)	( 86	8)	( 87	6)	( 88	3)	( 89	43)
( 90	4)	( 91	3)	( 93	3)	( 94	4)	( 95	9)
( 96	52)	( 97	23)	( 98	28)	( 99	11)	(100	7)
(101	15)	(102	7)	(103	197)	(104	19)	(105	13)
(106	4)	(107	9)	(108	4)	(110	4)	(111	7)
(112	6)	(113	13)	(114	8)	(115	6)	(116	7)
(117	58)	(118	6)	(119	7)	(122	5)	(123	11)
(124	3)	(125	4)	(126	6)	(127	6)	(128	16)
(129	42)	(130	6)	(131	19)	(132	3)	(133	52)
(134	7)	(135	11)	(136	6)	(138	3)	(139	3)
(140	7)	(141	7)	(142	24)	(143	13)	(144	6)
(145	4)	(147	207)	(148	32)	(149	21)	(150	5)
(151	3)	(152	4)	(153	3)	(154	6)	(155	7)
(156	99)	(157	23)	(158	11)	(159	3)	(160	5)
(161	3)	(163	6)	(166	3)	(167	5)	(168	7)
(169	4)	(170	21)	(171	4)	(172	6)	(173	36)
(174	4)	(175	4)	(177	3)	(179	3)	(180	3)
(181	6)	(182	4)	(183	5)	(184	3)	(185	3)
(186	61)	(187	11)	(188	4)	(189	19)	(190	5)
(191	8)	(192	3)	(195	3)	(196	3)	(197	4)
(198	6)	(202	4)	(203	3)	(204	13)	(205	27)
(206	6)	(207	6)	(209	4)	(213	5)	(214	51)
(215	8)	(216	5)	(217	68)	(218	14)	(219	6)
(221	5)	(224	3)	(225	13)	(226	4)	(229	3)
(230	6)	(237	6)	(244	7)	(246	4)	(253	3)
(255	3)	(258	3)	(269	3)	(270	3)	(274	6)
(275	3)	(277	3)	(287	3)	(291	3)	(299	6)
(300	3)	(307	6)	(313	7)	(319	3)	(327	4)
(343	14)	(344	6)	(345	4)	(346	10)	(347	4)
(355	4)	(356	3)	(372	3)	(373	10)	(374	11)
(375	5)	(411	3)	(414	3)	(415	15)	(416	11)
(417	9)	(444	3)	(445	16)	(446	65)	(447	28)
(448	11)								

NAME:12C\_2493.1\_1313EC75\_[657; Erythritol (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:249001-10-1

RI:2493

RT:15.316

NUM PEAKS: 236

( 72	14)	( 73	1000)	( 74	83)	( 75	95)	( 76	9)
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188

( 77	5)	( 80	5)	( 82	4)	( 84	6)	( 86	3)
( 87	14)	( 88	4)	( 89	37)	( 90	4)	( 93	5)
( 94	4)	( 95	7)	( 96	35)	( 97	6)	( 98	18)
(100	8)	(101	16)	(102	8)	(103	188)	(104	15)
(105	12)	(106	3)	(107	10)	(108	5)	(114	8)
(115	4)	(116	4)	(117	51)	(118	6)	(119	9)
(122	3)	(123	9)	(124	3)	(126	3)	(128	14)
(129	39)	(130	7)	(131	17)	(133	43)	(134	6)
(135	10)	(137	3)	(138	3)	(139	3)	(140	6)
(142	23)	(143	12)	(144	5)	(145	4)	(146	4)
(147	218)	(148	35)	(149	22)	(150	5)	(151	3)
(152	5)	(154	6)	(156	74)	(157	20)	(158	8)
(159	3)	(160	5)	(161	4)	(162	3)	(163	5)
(164	4)	(166	4)	(167	6)	(168	6)	(170	22)
(171	4)	(172	6)	(173	39)	(174	9)	(175	8)
(176	4)	(177	3)	(179	5)	(180	5)	(181	5)
(182	4)	(184	3)	(186	30)	(187	8)	(188	6)
(189	17)	(190	6)	(191	10)	(192	3)	(193	4)
(195	5)	(196	7)	(198	8)	(199	4)	(200	5)
(202	4)	(203	3)	(204	6)	(205	27)	(206	6)
(207	10)	(209	5)	(214	23)	(215	4)	(216	3)
(217	70)	(218	15)	(219	5)	(220	3)	(221	14)
(222	3)	(223	5)	(224	4)	(225	11)	(226	3)
(227	4)	(229	3)	(230	4)	(231	4)	(235	3)
(236	4)	(237	5)	(239	3)	(240	3)	(241	3)
(244	5)	(246	3)	(247	4)	(249	4)	(250	4)
(251	4)	(252	3)	(253	5)	(254	3)	(255	4)
(256	5)	(258	5)	(263	3)	(265	4)	(266	5)
(268	4)	(269	4)	(270	5)	(271	3)	(273	3)
(274	9)	(275	5)	(276	3)	(277	6)	(278	4)
(279	3)	(281	6)	(283	3)	(284	3)	(286	4)
(288	4)	(295	4)	(307	10)	(311	3)	(313	9)
(314	4)	(316	3)	(319	3)	(320	4)	(326	3)
(327	5)	(328	3)	(329	4)	(330	3)	(331	3)
(332	3)	(338	4)	(339	3)	(340	3)	(342	3)
(343	13)	(344	8)	(345	4)	(346	10)	(347	6)
(348	3)	(349	3)	(351	3)	(355	5)	(356	4)
(362	3)	(367	3)	(372	3)	(373	18)	(374	14)
(375	6)	(376	4)	(378	3)	(380	3)	(391	3)
(395	3)	(398	3)	(406	3)	(411	3)	(412	3)
(414	5)	(415	17)	(416	12)	(417	7)	(418	4)
(423	3)	(429	3)	(430	3)	(431	4)	(437	4)
(438	3)	(442	3)	(443	4)	(444	3)	(445	20)
(446	69)	(447	32)	(448	13)	(449	5)	(457	3)
(461	3)	(462	3)	(468	3)	(469	4)	(486	3)
(515	3)	(522	4)	(534	3)	(539	3)	(540	3)
(543	3)								

NAME:12C\_2134.7\_1274EC17\_[904; Galactose methoxyamine (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:214003-10-1

RI:2135

RT:13.842

NUM PEAKS: 108

( 70	5)	( 72	15)	( 73	1000)	( 74	79)	( 75	66)
( 83	16)	( 84	20)	( 87	5)	( 89	48)	( 90	6)
( 92	3)	(100	12)	(101	13)	(102	5)	(103	217)
(104	20)	(105	11)	(112	3)	(113	7)	(114	10)
(115	6)	(116	4)	(117	82)	(118	8)	(119	8)
(120	3)	(127	4)	(129	97)	(130	15)	(131	24)

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(133	98)	(134	12)	(135	8)	(138	3)	(141	4)
(142	5)	(143	12)	(147	261)	(148	40)	(149	23)
(150	3)	(155	4)	(156	3)	(157	111)	(158	15)
(159	10)	(163	10)	(166	4)	(171	3)	(172	29)
(173	18)	(174	5)	(175	6)	(177	5)	(189	29)
(190	11)	(191	17)	(193	4)	(200	3)	(201	9)
(202	5)	(203	5)	(204	27)	(205	168)	(206	32)
(207	16)	(214	3)	(216	5)	(217	112)	(218	23)
(219	9)	(227	3)	(229	27)	(230	11)	(231	8)
(232	3)	(233	4)	(235	4)	(243	3)	(244	3)
(245	4)	(247	3)	(257	3)	(260	3)	(262	8)
(263	7)	(268	5)	(271	4)	(272	4)	(273	4)
(274	4)	(277	5)	(288	4)	(291	7)	(302	4)
(305	7)	(306	5)	(307	8)	(318	3)	(319	217)
(320	68)	(321	33)	(322	6)	(332	6)	(333	3)
(378	3)	(402	4)	(514	4)				

NAME:12C\_2128.7\_1274EC17\_[857; Mannitol (6TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:213001-10-1

RI:2129

RT:13.804

NUM PEAKS: 237

( 70	18)	( 71	81)	( 72	20)	( 73	1000)	( 74	82)
( 75	77)	( 76	6)	( 77	5)	( 79	3)	( 80	6)
( 81	13)	( 82	15)	( 83	59)	( 84	48)	( 85	60)
( 86	9)	( 87	6)	( 88	6)	( 89	52)	( 90	5)
( 92	3)	( 93	19)	( 94	6)	( 95	12)	( 96	4)
( 97	41)	( 98	8)	( 99	28)	(100	7)	(101	15)
(102	5)	(103	200)	(104	21)	(105	21)	(106	5)
(110	4)	(111	25)	(112	9)	(113	21)	(114	28)
(115	9)	(116	5)	(117	71)	(118	7)	(119	12)
(120	3)	(121	3)	(123	11)	(125	16)	(126	6)
(127	17)	(128	5)	(129	103)	(130	24)	(131	25)
(133	66)	(134	10)	(135	10)	(138	4)	(139	5)
(140	5)	(141	10)	(142	9)	(143	16)	(144	5)
(146	12)	(147	261)	(148	39)	(149	29)	(150	4)
(151	4)	(152	4)	(153	5)	(154	5)	(155	10)
(156	4)	(157	112)	(158	17)	(159	6)	(160	3)
(161	4)	(162	4)	(163	14)	(164	3)	(165	3)
(167	3)	(168	5)	(169	6)	(170	6)	(171	3)
(172	8)	(173	13)	(175	5)	(176	3)	(177	5)
(180	4)	(181	5)	(182	4)	(183	3)	(184	5)
(185	4)	(186	3)	(187	3)	(188	5)	(189	29)
(190	10)	(191	21)	(192	6)	(198	6)	(200	3)
(201	5)	(202	8)	(203	7)	(204	31)	(205	167)
(206	33)	(207	14)	(210	3)	(211	4)	(214	4)
(215	6)	(216	7)	(217	116)	(218	24)	(219	11)
(220	6)	(224	3)	(228	3)	(229	26)	(230	12)
(231	9)	(232	4)	(233	4)	(238	4)	(240	4)
(242	4)	(243	5)	(244	4)	(245	3)	(246	4)
(247	3)	(248	3)	(254	4)	(255	3)	(256	3)
(257	4)	(262	34)	(263	13)	(264	5)	(266	4)
(270	3)	(271	3)	(275	3)	(277	7)	(278	6)
(280	4)	(284	3)	(288	5)	(289	3)	(290	4)
(291	9)	(292	4)	(304	4)	(305	6)	(306	3)
(307	8)	(308	5)	(309	3)	(311	3)	(312	4)
(313	3)	(318	6)	(319	227)	(320	73)	(321	31)
(322	7)	(323	4)	(330	3)	(331	5)	(332	3)
(333	4)	(334	6)	(335	4)	(336	6)	(337	4)

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(338	3)	(339	4)	(340	3)	(342	3)	(344	3)
(345	3)	(347	3)	(352	4)	(358	3)	(364	4)
(368	3)	(374	4)	(376	4)	(377	3)	(380	4)
(381	3)	(386	3)	(390	3)	(391	3)	(392	3)
(393	3)	(400	3)	(401	4)	(402	5)	(404	3)
(405	3)	(407	3)	(419	3)	(436	3)	(437	3)
(446	4)	(457	3)	(459	3)	(464	3)	(466	4)
(467	3)	(476	3)	(484	3)	(485	3)	(486	3)
(488	3)	(489	3)	(500	3)	(504	3)	(508	3)
(512	3)	(513	3)	(515	3)	(516	3)	(518	3)
(528	4)	(548	3)						

NAME:12C\_2217.8\_1274EC17\_9-(Z)-Octadecenoic acid (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:222001-10-1

RI:2218

RT:14.350

NUM PEAKS: 146

( 70	43)	( 71	11)	( 72	39)	( 73	838)	( 74	88)
( 75	1000)	( 76	67)	( 77	66)	( 78	11)	( 79	84)
( 80	36)	( 81	189)	( 82	96)	( 83	144)	( 84	190)
( 85	26)	( 86	9)	( 87	7)	( 88	6)	( 89	27)
( 90	3)	( 91	28)	( 92	9)	( 93	49)	( 94	34)
( 95	140)	( 96	230)	( 97	128)	( 98	156)	( 99	29)
(101	10)	(102	3)	(103	3)	(105	30)	(106	8)
(107	27)	(108	22)	(109	75)	(110	86)	(111	58)
(112	31)	(113	5)	(116	27)	(117	731)	(118	73)
(119	53)	(120	8)	(121	34)	(122	11)	(123	57)
(124	37)	(125	21)	(126	6)	(128	5)	(129	552)
(130	70)	(131	105)	(132	135)	(133	56)	(134	27)
(135	17)	(136	6)	(137	41)	(138	31)	(139	11)
(140	4)	(141	3)	(142	4)	(143	38)	(144	7)
(145	243)	(146	33)	(147	35)	(148	16)	(149	13)
(150	5)	(151	26)	(152	41)	(153	7)	(155	26)
(156	7)	(157	16)	(158	8)	(159	20)	(160	3)
(161	7)	(162	4)	(163	4)	(164	4)	(165	14)
(166	23)	(167	8)	(168	3)	(169	16)	(170	9)
(171	26)	(172	10)	(173	11)	(174	5)	(175	4)
(179	6)	(180	34)	(181	6)	(183	21)	(184	6)
(185	59)	(186	14)	(187	11)	(188	5)	(193	4)
(194	5)	(199	80)	(200	14)	(201	13)	(206	3)
(207	8)	(208	3)	(213	11)	(214	3)	(217	14)
(218	7)	(220	10)	(221	10)	(222	44)	(223	9)
(227	4)	(235	5)	(236	7)	(241	8)	(246	4)
(255	3)	(257	5)	(258	3)	(264	34)	(265	8)
(272	4)	(294	4)	(295	9)	(296	3)	(311	3)
(338	3)	(339	112)	(340	40)	(341	9)	(354	14)
(355	5)								

NAME:12C\_2278.6\_1274EC17\_[583; Erythritol (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:228001-10-1

RI:2279

RT:14.672

NUM PEAKS: 235

( 70	4)	( 71	45)	( 72	28)	( 73	1000)	( 74	86)
( 75	49)	( 77	27)	( 78	15)	( 79	33)	( 80	21)
( 81	24)	( 85	15)	( 87	9)	( 89	27)	( 91	32)
( 92	21)	( 93	66)	( 94	12)	( 98	5)	(100	9)
(101	6)	(102	3)	(103	77)	(105	24)	(113	5)

191

(114	8)	(117	74)	(122	9)	(126	10)	(128	10)
(129	20)	(131	17)	(133	131)	(134	61)	(137	3)
(139	6)	(140	7)	(142	9)	(143	6)	(144	5)
(145	4)	(147	194)	(148	40)	(149	18)	(150	9)
(151	9)	(152	9)	(153	6)	(154	3)	(157	16)
(158	5)	(159	8)	(163	6)	(164	3)	(165	7)
(168	7)	(170	5)	(172	12)	(173	12)	(176	3)
(180	4)	(183	12)	(186	13)	(188	5)	(189	21)
(190	19)	(191	12)	(194	7)	(197	4)	(199	11)
(201	34)	(202	15)	(204	13)	(205	45)	(206	11)
(212	8)	(213	3)	(214	21)	(215	7)	(216	8)
(217	58)	(218	19)	(219	4)	(222	3)	(224	5)
(226	15)	(227	7)	(229	9)	(230	4)	(231	6)
(233	7)	(234	15)	(235	8)	(236	4)	(241	6)
(243	4)	(244	9)	(245	7)	(246	24)	(247	8)
(248	6)	(251	3)	(252	6)	(254	13)	(256	5)
(257	4)	(258	4)	(260	11)	(265	5)	(266	7)
(267	4)	(268	12)	(269	11)	(270	5)	(274	3)
(275	9)	(278	7)	(282	4)	(284	10)	(285	4)
(286	9)	(287	4)	(288	3)	(289	8)	(290	149)
(291	42)	(292	18)	(293	10)	(294	11)	(295	3)
(296	6)	(301	5)	(306	3)	(307	4)	(308	5)
(310	5)	(315	5)	(316	6)	(317	5)	(319	36)
(320	15)	(325	6)	(327	4)	(331	8)	(335	3)
(336	5)	(346	5)	(347	9)	(348	5)	(352	5)
(354	6)	(355	7)	(356	4)	(359	4)	(360	5)
(361	3)	(364	6)	(365	8)	(367	8)	(368	4)
(369	4)	(374	4)	(380	6)	(381	3)	(382	3)
(383	5)	(384	5)	(385	6)	(387	12)	(388	10)
(389	3)	(390	5)	(392	3)	(393	3)	(394	3)
(395	3)	(404	8)	(405	6)	(406	3)	(409	5)
(410	4)	(411	3)	(412	7)	(413	5)	(414	4)
(416	7)	(421	7)	(422	3)	(424	9)	(425	9)
(428	3)	(430	8)	(431	5)	(433	6)	(434	3)
(437	3)	(440	5)	(445	4)	(448	4)	(452	5)
(453	5)	(462	4)	(465	6)	(468	5)	(473	4)
(476	4)	(477	4)	(481	5)	(483	3)	(486	6)
(489	10)	(492	5)	(494	3)	(498	4)	(499	5)
(504	5)	(513	4)	(521	8)	(522	10)	(524	3)
(525	10)	(530	4)	(535	3)	(538	7)	(539	4)
(541	8)	(542	4)	(543	3)	(545	3)	(549	6)
(550	3)	(556	6)	(567	3)	(571	3)	(590	3)

NAME:12C\_2294.6\_1274EC17\_[877; beta-D-Galactopyranoside-(1,2)-glycerol  
(6TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:230001-10-1

RI:2295

RT:14.757

NUM PEAKS: 71

( 73	1000)	( 74	70)	( 75	80)	( 78	15)	( 87	12)
( 89	11)	(101	47)	(103	223)	(104	21)	(116	10)
(117	53)	(118	11)	(129	115)	(130	32)	(131	42)
(133	29)	(134	15)	(135	15)	(143	10)	(147	207)
(148	42)	(149	19)	(154	17)	(161	9)	(163	8)
(189	29)	(191	72)	(192	19)	(202	10)	(203	32)
(204	676)	(205	142)	(206	48)	(217	119)	(218	42)
(219	50)	(223	7)	(231	21)	(232	10)	(240	8)
(242	8)	(243	17)	(258	6)	(274	15)	(280	6)
(281	15)	(286	8)	(293	10)	(295	8)	(296	13)

192

(297	9)	(298	9)	(303	12)	(319	14)	(324	9)
(331	12)	(337	70)	(338	25)	(359	8)	(382	7)
(383	7)	(414	10)	(450	11)	(464	7)	(489	18)
(493	16)	(494	9)	(511	9)	(512	13)	(574	4)
(579	4)								

NAME:12C\_2311.4\_1274EC17\_Galactose-6-phosphate methoxyamine (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:232001-10-1

RI:2311

RT:14.846

NUM PEAKS: 321

( 70	43)	( 71	90)	( 72	74)	( 73	1000)	( 74	112)
( 75	212)	( 76	6)	( 82	7)	( 84	27)	( 86	15)
( 87	21)	( 88	19)	( 89	37)	( 90	8)	( 96	14)
( 98	9)	(100	24)	(101	135)	(102	17)	(110	10)
(112	21)	(113	6)	(114	19)	(116	13)	(124	14)
(129	12)	(130	45)	(140	6)	(144	17)	(147	237)
(148	22)	(149	11)	(150	14)	(157	46)	(158	27)
(160	159)	(162	6)	(163	11)	(166	3)	(168	7)
(169	12)	(174	8)	(175	8)	(177	10)	(178	11)
(179	16)	(181	13)	(182	20)	(183	4)	(184	6)
(189	5)	(191	27)	(192	14)	(193	13)	(195	13)
(196	19)	(197	6)	(203	4)	(204	18)	(205	18)
(206	21)	(207	35)	(208	7)	(209	13)	(210	5)
(211	39)	(212	17)	(216	17)	(217	23)	(218	10)
(220	21)	(221	23)	(222	21)	(223	10)	(224	8)
(225	8)	(228	13)	(229	14)	(230	8)	(231	21)
(232	10)	(233	15)	(234	15)	(235	8)	(238	2)
(242	5)	(245	5)	(246	10)	(247	19)	(248	3)
(249	9)	(250	15)	(251	18)	(252	9)	(253	17)
(254	14)	(255	12)	(256	5)	(257	10)	(258	3)
(261	9)	(262	9)	(263	15)	(264	11)	(265	15)
(266	4)	(267	9)	(270	4)	(271	5)	(272	8)
(273	3)	(274	9)	(277	12)	(278	4)	(279	9)
(280	8)	(281	14)	(282	10)	(283	8)	(284	7)
(285	17)	(286	9)	(287	9)	(289	6)	(290	5)
(291	10)	(292	7)	(293	3)	(294	6)	(295	13)
(297	5)	(298	6)	(299	130)	(300	36)	(301	21)
(302	17)	(303	18)	(304	7)	(305	9)	(306	7)
(307	8)	(308	12)	(309	2)	(313	6)	(314	6)
(316	5)	(319	9)	(323	9)	(324	7)	(325	10)
(326	5)	(328	161)	(329	79)	(330	10)	(331	29)
(332	3)	(336	6)	(337	13)	(339	8)	(340	5)
(341	10)	(342	8)	(343	8)	(345	4)	(347	2)
(352	11)	(353	6)	(354	15)	(355	11)	(356	4)
(357	51)	(358	21)	(359	21)	(360	6)	(362	2)
(363	3)	(364	8)	(365	5)	(368	8)	(369	6)
(370	7)	(371	18)	(373	5)	(374	12)	(377	10)
(378	4)	(379	13)	(380	11)	(382	12)	(386	23)
(387	220)	(388	103)	(389	47)	(390	7)	(392	11)
(394	10)	(395	11)	(396	10)	(397	14)	(398	8)
(399	3)	(402	7)	(403	9)	(404	14)	(405	15)
(406	6)	(407	9)	(408	4)	(412	5)	(413	11)
(414	9)	(415	4)	(416	15)	(417	13)	(423	8)
(424	11)	(425	11)	(427	3)	(429	12)	(433	5)
(434	6)	(436	13)	(437	7)	(438	4)	(439	5)
(441	5)	(442	4)	(443	15)	(444	9)	(446	10)
(447	5)	(448	6)	(449	17)	(450	6)	(451	5)
(452	4)	(453	3)	(454	9)	(455	4)	(457	8)

193

(458	11)	(461	10)	(462	5)	(464	5)	(465	8)
(466	9)	(469	13)	(470	3)	(471	21)	(472	25)
(473	20)	(474	6)	(475	3)	(476	12)	(477	5)
(478	10)	(480	5)	(483	2)	(484	13)	(485	11)
(486	5)	(487	4)	(489	6)	(490	10)	(491	9)
(492	4)	(493	6)	(496	14)	(498	4)	(501	10)
(502	6)	(504	18)	(505	6)	(507	22)	(508	10)
(511	8)	(514	4)	(515	12)	(516	3)	(518	6)
(522	6)	(523	5)	(524	2)	(525	7)	(528	2)
(529	12)	(531	2)	(532	8)	(533	2)	(534	4)
(535	4)	(538	2)	(539	4)	(540	6)	(541	2)
(542	5)	(543	16)	(547	5)	(549	2)	(550	4)
(552	5)	(553	3)	(559	2)	(564	2)	(565	2)
(566	5)	(568	11)	(569	5)	(571	2)	(572	1)
(574	2)	(575	5)	(580	3)	(581	1)	(585	2)
(586	2)	(588	4)	(590	1)	(593	3)	(596	2)
(598	1)								

NAME:12C\_2474.9\_1274EC17\_[945; Uridine (3TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:248002-10-1

RI:2475

RT:15.711

NUM PEAKS: 131

( 70	12)	( 71	8)	( 72	22)	( 73	1000)	( 74	84)
( 75	136)	( 76	9)	( 77	10)	( 79	3)	( 81	8)
( 82	6)	( 83	4)	( 84	4)	( 85	13)	( 86	4)
( 87	7)	( 89	16)	( 94	3)	( 95	5)	( 96	8)
( 97	14)	( 98	5)	( 99	49)	(100	14)	(101	28)
(102	7)	(103	175)	(104	16)	(105	9)	(110	3)
(111	9)	(112	4)	(113	19)	(114	4)	(115	39)
(116	11)	(117	29)	(118	3)	(119	8)	(124	4)
(125	5)	(126	10)	(127	10)	(128	4)	(129	74)
(130	10)	(131	26)	(132	4)	(133	68)	(134	9)
(135	8)	(137	3)	(138	5)	(140	6)	(141	7)
(142	7)	(143	33)	(144	5)	(145	8)	(147	171)
(148	47)	(149	36)	(150	5)	(151	3)	(153	15)
(154	6)	(155	6)	(156	4)	(157	13)	(158	3)
(159	5)	(163	7)	(167	3)	(168	11)	(169	154)
(170	23)	(171	15)	(173	3)	(174	3)	(175	3)
(177	4)	(183	12)	(184	3)	(185	32)	(186	5)
(187	3)	(189	17)	(190	4)	(191	46)	(192	7)
(203	8)	(204	10)	(205	4)	(211	12)	(213	28)
(214	4)	(215	17)	(216	5)	(217	420)	(218	102)
(219	45)	(220	6)	(226	6)	(227	5)	(229	5)
(230	24)	(231	21)	(232	5)	(239	3)	(241	5)
(243	52)	(244	11)	(245	21)	(246	4)	(251	3)
(257	7)	(258	5)	(259	91)	(260	20)	(261	8)
(265	15)	(267	8)	(280	3)	(299	16)	(300	5)
(315	9)	(316	3)	(317	4)	(348	3)	(349	3)
(445	5)								

NAME:12C\_2687.5\_1274EC17\_[964; Trehalose (8TMS); alpha-D-Glc-(1,1)-alpha-D-Glc]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:269002-10-1

RI:2688

RT:16.837

NUM PEAKS: 93

( 72	12)	( 73	1000)	( 74	84)	( 75	76)	( 81	20)
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194

( 94	6)	(101	13)	(103	160)	(104	15)	(107	5)
(113	9)	(115	8)	(116	18)	(117	58)	(127	10)
(129	146)	(130	17)	(131	30)	(133	53)	(135	9)
(142	8)	(143	23)	(144	8)	(145	9)	(147	232)
(148	38)	(149	31)	(153	7)	(155	26)	(157	26)
(158	10)	(163	7)	(169	122)	(170	19)	(171	13)
(177	6)	(181	9)	(183	6)	(189	31)	(190	11)
(191	261)	(192	40)	(193	23)	(199	8)	(203	13)
(204	84)	(205	33)	(207	12)	(211	5)	(217	171)
(218	39)	(219	18)	(229	14)	(230	11)	(231	15)
(233	7)	(242	4)	(243	47)	(244	15)	(245	10)
(257	6)	(258	5)	(259	7)	(265	4)	(271	46)
(272	11)	(273	9)	(282	3)	(287	6)	(291	7)
(292	5)	(319	16)	(320	12)	(321	6)	(331	23)
(332	13)	(361	246)	(362	84)	(363	42)	(364	12)
(374	6)	(387	3)	(435	7)	(451	8)	(452	4)
(455	5)	(456	3)	(461	5)	(507	4)	(512	4)
(524	4)	(528	5)	(574	3)				

NAME:12C\_2748.2\_1274EC17\_Trehalose (8TMS); alpha-D-Glc-(1,1)-alpha-D-Glc

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:274002-10-1

RI:2748

RT:17.158

NUM PEAKS: 213

( 70	2)	( 71	3)	( 72	11)	( 73	1000)	( 74	89)
( 75	89)	( 76	5)	( 77	4)	( 79	1)	( 80	1)
( 81	23)	( 82	2)	( 83	5)	( 84	1)	( 85	8)
( 86	1)	( 87	6)	( 88	2)	( 89	15)	( 90	2)
( 91	2)	( 94	1)	( 95	2)	( 97	4)	( 98	1)
( 99	7)	(100	1)	(101	20)	(102	5)	(103	243)
(104	23)	(105	11)	(109	12)	(110	1)	(111	5)
(112	1)	(113	13)	(114	4)	(115	9)	(116	12)
(117	67)	(118	7)	(119	8)	(120	1)	(125	1)
(126	1)	(127	7)	(128	2)	(129	192)	(130	24)
(131	39)	(132	6)	(133	52)	(134	8)	(135	5)
(139	4)	(140	1)	(141	5)	(142	6)	(143	26)
(144	4)	(145	9)	(146	2)	(147	287)	(148	45)
(149	37)	(150	5)	(151	3)	(153	5)	(154	2)
(155	28)	(156	6)	(157	26)	(158	4)	(159	5)
(160	1)	(161	4)	(162	1)	(163	6)	(164	1)
(165	1)	(167	2)	(168	1)	(169	142)	(170	24)
(171	13)	(172	2)	(173	8)	(174	2)	(175	5)
(176	1)	(177	5)	(178	1)	(179	1)	(181	2)
(182	1)	(183	6)	(184	1)	(185	2)	(187	2)
(189	23)	(190	7)	(191	347)	(192	66)	(193	31)
(194	4)	(195	1)	(199	4)	(200	1)	(201	3)
(202	3)	(203	12)	(204	98)	(205	37)	(206	12)
(207	7)	(208	1)	(215	5)	(216	2)	(217	177)
(218	47)	(219	22)	(220	4)	(221	12)	(222	3)
(223	2)	(227	4)	(228	2)	(229	16)	(230	10)
(231	15)	(232	5)	(233	10)	(234	3)	(235	1)
(239	1)	(241	6)	(242	3)	(243	59)	(244	18)
(245	17)	(246	4)	(247	5)	(248	1)	(249	1)
(255	3)	(256	1)	(257	7)	(258	2)	(259	6)
(260	2)	(261	1)	(263	6)	(264	1)	(265	5)
(266	1)	(267	1)	(270	1)	(271	71)	(272	18)
(273	11)	(274	2)	(275	1)	(277	1)	(278	1)
(279	7)	(280	2)	(281	1)	(287	2)	(288	1)
(289	1)	(290	9)	(291	12)	(292	5)	(293	3)



195

(303	1)	(304	1)	(305	9)	(306	4)	(307	3)
(308	1)	(317	4)	(318	3)	(319	22)	(320	11)
(321	5)	(322	2)	(323	3)	(324	1)	(331	22)
(332	14)	(333	8)	(334	3)	(335	1)	(345	2)
(346	2)	(347	1)	(360	8)	(361	120)	(362	66)
(363	29)	(364	7)	(365	2)	(377	3)	(378	1)
(379	1)	(393	1)	(407	1)	(408	1)	(435	3)
(451	5)	(463	2)	(464	1)				

NAME:12C\_2929.8\_1274EC17\_[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:293001-10-1

RI:2930

RT:18.009

NUM PEAKS: 124

( 70	4)	( 71	5)	( 72	10)	( 73	1000)	( 74	85)
( 75	81)	( 76	4)	( 77	6)	( 79	3)	( 81	20)
( 83	6)	( 85	5)	( 87	5)	( 89	8)	( 97	4)
( 99	5)	(101	14)	(102	4)	(103	136)	(104	13)
(105	6)	(109	7)	(111	4)	(113	7)	(115	5)
(116	11)	(117	40)	(118	4)	(119	5)	(127	5)
(129	146)	(130	17)	(131	28)	(132	4)	(133	51)
(134	7)	(135	5)	(139	3)	(141	4)	(142	4)
(143	27)	(144	4)	(145	6)	(147	276)	(148	43)
(149	31)	(150	4)	(151	3)	(153	5)	(155	11)
(156	3)	(157	19)	(158	3)	(159	4)	(161	5)
(163	4)	(169	38)	(170	8)	(171	6)	(173	4)
(175	5)	(177	6)	(181	3)	(183	4)	(189	26)
(190	10)	(191	223)	(192	39)	(193	18)	(201	3)
(203	12)	(204	808)	(205	166)	(206	70)	(207	18)
(208	3)	(215	5)	(217	159)	(218	37)	(219	17)
(220	3)	(221	21)	(222	5)	(223	3)	(229	6)
(230	24)	(231	14)	(232	4)	(233	5)	(239	3)
(242	3)	(243	25)	(244	7)	(245	7)	(246	3)
(255	3)	(257	4)	(265	6)	(271	14)	(272	3)
(291	9)	(292	3)	(293	9)	(295	3)	(304	6)
(305	24)	(306	9)	(307	4)	(317	4)	(318	14)
(319	12)	(320	4)	(331	5)	(332	8)	(333	4)
(343	7)	(344	3)	(345	5)	(361	29)	(362	11)
(363	5)	(433	16)	(434	8)	(435	5)		

NAME:12C\_3337.9\_1191EC10\_[700; Ergosta-5,7-dien-3-ol]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:334001-10-1

RI:3338

RT:19.741

NUM PEAKS: 90

( 70	66)	( 71	155)	( 73	1000)	( 74	85)	( 75	887)
( 76	70)	( 77	108)	( 81	244)	( 83	108)	( 89	18)
( 90	13)	( 91	157)	( 93	130)	( 94	21)	( 95	155)
( 97	52)	(100	17)	(101	47)	(105	118)	(107	68)
(109	72)	(111	20)	(115	78)	(116	29)	(117	80)
(119	132)	(121	45)	(123	21)	(128	65)	(129	198)
(130	44)	(131	160)	(132	32)	(133	57)	(135	27)
(141	57)	(142	37)	(143	165)	(144	73)	(145	129)
(146	37)	(149	20)	(151	19)	(153	20)	(154	14)
(155	91)	(156	31)	(157	88)	(158	51)	(159	85)
(160	12)	(161	29)	(165	29)	(167	18)	(168	15)
(169	55)	(170	21)	(171	63)	(172	18)	(173	27)

196

(180	10)	(181	27)	(183	45)	(185	40)	(187	18)
(193	28)	(195	21)	(196	16)	(197	51)	(200	16)
(201	23)	(207	44)	(211	52)	(212	17)	(213	24)
(221	58)	(222	21)	(225	17)	(239	25)	(242	13)
(251	17)	(253	20)	(339	51)	(340	23)	(341	12)
(365	61)	(366	22)	(371	12)	(380	20)	(471	14)

NAME:12C\_3350.3\_1274EC11\_[692; Ergosta-7,22-dien-3-ol (1TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:335001-10-1

RI:3350

RT:19.858

NUM PEAKS: 159

( 70	48)	( 73	599)	( 74	60)	( 75	1000)	( 76	89)
( 77	162)	( 78	65)	( 79	292)	( 80	38)	( 81	278)
( 82	29)	( 83	118)	( 86	22)	( 87	26)	( 89	39)
( 91	298)	( 92	55)	( 93	223)	( 94	59)	( 95	174)
( 97	22)	(101	35)	(103	68)	(104	19)	(105	281)
(106	53)	(107	280)	(108	54)	(109	83)	(114	26)
(115	103)	(116	23)	(117	131)	(118	13)	(119	152)
(120	50)	(121	120)	(123	41)	(124	36)	(127	26)
(128	36)	(129	110)	(130	34)	(131	159)	(132	59)
(133	144)	(134	47)	(135	55)	(141	29)	(142	34)
(143	77)	(144	28)	(145	154)	(146	67)	(147	254)
(148	44)	(149	55)	(150	97)	(151	23)	(153	18)
(155	48)	(156	20)	(157	86)	(159	143)	(160	45)
(161	49)	(164	58)	(169	63)	(171	75)	(172	24)
(173	62)	(174	22)	(175	33)	(177	21)	(183	35)
(185	62)	(186	29)	(187	32)	(188	13)	(189	37)
(195	18)	(197	23)	(199	45)	(201	33)	(202	27)
(203	22)	(205	22)	(209	30)	(210	18)	(211	70)
(213	92)	(216	21)	(219	16)	(220	20)	(222	22)
(226	19)	(227	91)	(228	27)	(232	15)	(239	22)
(241	14)	(248	20)	(251	20)	(253	101)	(254	25)
(267	24)	(281	50)	(282	33)	(283	22)	(284	17)
(290	13)	(295	17)	(301	20)	(303	11)	(307	21)
(314	16)	(315	18)	(321	12)	(329	21)	(330	16)
(342	17)	(343	272)	(344	122)	(345	40)	(360	15)
(365	25)	(366	16)	(371	35)	(372	25)	(375	15)
(378	23)	(380	18)	(386	91)	(387	55)	(388	25)
(389	13)	(404	21)	(417	18)	(433	20)	(443	15)
(444	16)	(446	14)	(455	37)	(456	14)	(457	13)
(470	22)	(471	19)	(481	13)	(486	17)	(492	13)
(504	18)	(509	13)	(513	16)	(520	16)	(545	7)
(546	11)	(569	9)	(580	5)	(592	4)		

NAME:12C\_3358.2\_1191EC08\_[693; Ergost-7-en-3-ol (1TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:335002-10-1

RI:3358

RT:19.826

NUM PEAKS: 48

( 71	242)	( 73	477)	( 75	1000)	( 76	93)	( 79	205)
( 81	185)	( 83	74)	( 91	269)	( 92	92)	( 93	167)
( 94	47)	( 95	217)	( 96	51)	( 97	68)	(105	281)
(106	64)	(107	179)	(108	54)	(109	80)	(111	23)
(117	104)	(119	154)	(120	45)	(121	86)	(123	35)
(128	32)	(131	153)	(133	113)	(134	43)	(143	40)
(145	123)	(147	174)	(159	82)	(161	67)	(173	29)
(201	39)	(213	147)	(214	40)	(229	53)	(255	159)

197

(256 39) (273 19) (306 27) (307 19) (367 21)  
 (471 15) (472 68) (473 40)

NAME:12C\_3401.9\_1274EC11\_[805; 4,4-Dimethylcholesta-8,24-dien-3-ol (1TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:340002-10-1

RI:3402

RT:20.078

NUM PEAKS: 112

( 73 1000) ( 74 69) ( 75 649) ( 79 223) ( 81 364)  
 ( 82 80) ( 87 36) ( 89 31) ( 91 278) ( 92 47)  
 ( 93 269) ( 94 53) ( 95 377) (104 17) (105 290)  
 (106 59) (107 286) (108 56) (109 265) (117 147)  
 (119 264) (120 73) (121 183) (122 80) (123 130)  
 (124 31) (128 35) (129 273) (131 178) (132 120)  
 (133 228) (134 116) (135 775) (136 181) (137 84)  
 (143 115) (144 54) (145 235) (146 128) (148 68)  
 (149 188) (150 29) (152 34) (154 12) (156 29)  
 (157 112) (158 33) (159 149) (160 66) (161 137)  
 (162 40) (163 85) (169 26) (171 101) (172 31)  
 (173 126) (174 75) (175 140) (176 38) (177 50)  
 (183 41) (185 67) (186 29) (187 144) (188 61)  
 (189 58) (190 29) (197 24) (199 61) (200 17)  
 (201 49) (203 58) (211 62) (213 30) (215 48)  
 (216 29) (225 69) (226 29) (229 50) (231 16)  
 (241 113) (242 20) (243 65) (255 23) (257 36)  
 (258 80) (259 27) (260 9) (278 14) (295 39)  
 (296 27) (325 24) (326 23) (351 42) (366 12)  
 (379 87) (380 53) (394 47) (396 17) (402 21)  
 (467 15) (471 30) (474 11) (484 76) (485 71)  
 (486 22) (491 23) (513 31) (540 16) (571 8)  
 (590 9) (592 4)

NAME:12C\_3487.5\_1191EC08\_[568; 2,3-Dihexadecanoylglycerol (1TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:349001-10-1

RI:3488

RT:20.373

NUM PEAKS: 103

( 70 57) ( 73 1000) ( 74 42) ( 75 286) ( 79 113)  
 ( 81 88) ( 83 102) ( 84 41) ( 86 8) ( 91 29)  
 ( 95 138) ( 97 49) ( 98 64) (101 46) (102 23)  
 (103 242) (104 27) (105 18) (106 20) (107 20)  
 (109 105) (115 33) (116 21) (117 84) (123 15)  
 (126 7) (128 25) (129 629) (130 84) (131 115)  
 (134 12) (135 41) (139 9) (142 13) (143 19)  
 (145 456) (146 66) (147 26) (148 11) (149 32)  
 (157 22) (159 9) (167 11) (168 21) (173 28)  
 (174 10) (178 15) (182 18) (183 122) (184 7)  
 (189 37) (193 33) (194 27) (201 27) (208 6)  
 (219 29) (220 19) (224 24) (227 5) (237 13)  
 (239 16) (243 5) (255 9) (257 194) (258 35)  
 (259 19) (273 57) (274 16) (275 15) (277 9)  
 (295 14) (296 10) (297 9) (300 7) (311 13)  
 (312 13) (313 100) (314 16) (315 23) (327 25)  
 (328 14) (329 30) (347 6) (348 6) (371 18)  
 (384 11) (385 32) (390 5) (409 17) (424 11)  
 (428 6) (433 28) (434 31) (469 11) (474 12)  
 (538 7) (551 18) (556 6) (569 17) (572 15)  
 (578 18) (579 10) (586 8)

NAME:12C\_3301.9\_1274EC11\_[674; Ergosterol (1TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:331001-10-1

RI:3302

RT:19.651

NUM PEAKS: 335

( 70 165)	( 71 742)	( 72 81)	( 73 1000)	( 74 130)
( 75 788)	( 76 91)	( 77 121)	( 79 95)	( 80 18)
( 81 367)	( 82 46)	( 83 329)	( 84 153)	( 85 340)
( 86 21)	( 87 23)	( 88 3)	( 89 52)	( 90 27)
( 91 132)	( 93 113)	( 95 285)	( 96 79)	( 97 133)
( 98 50)	( 99 141)	(100 43)	(101 51)	(102 27)
(103 261)	(104 11)	(105 102)	(106 47)	(107 82)
(108 11)	(109 80)	(110 36)	(111 44)	(112 34)
(113 76)	(115 111)	(116 69)	(117 198)	(118 39)
(119 107)	(120 25)	(121 73)	(122 20)	(123 42)
(124 23)	(125 63)	(126 31)	(127 63)	(128 71)
(129 969)	(130 185)	(131 357)	(132 69)	(133 123)
(135 25)	(136 25)	(137 58)	(139 27)	(140 3)
(141 134)	(142 73)	(143 198)	(144 70)	(145 990)
(146 151)	(147 55)	(151 5)	(152 30)	(153 30)
(154 64)	(155 379)	(156 70)	(157 204)	(158 62)
(159 138)	(160 43)	(161 18)	(162 9)	(163 7)
(165 53)	(166 13)	(167 48)	(168 24)	(169 114)
(170 29)	(171 93)	(172 35)	(173 17)	(174 6)
(176 13)	(177 11)	(178 16)	(180 26)	(181 83)
(182 38)	(183 98)	(184 31)	(185 62)	(187 24)
(188 42)	(189 74)	(190 16)	(191 21)	(193 6)
(194 10)	(195 76)	(196 37)	(197 79)	(198 22)
(199 72)	(200 25)	(201 35)	(207 26)	(209 42)
(210 45)	(211 89)	(212 32)	(213 76)	(214 40)
(215 25)	(216 12)	(218 18)	(219 7)	(222 16)
(223 37)	(224 24)	(225 27)	(226 14)	(227 37)
(228 25)	(229 376)	(230 86)	(231 27)	(232 7)
(235 15)	(237 52)	(238 33)	(239 53)	(240 18)
(241 3)	(243 9)	(245 31)	(246 22)	(247 16)
(248 16)	(250 9)	(251 33)	(252 16)	(253 126)
(254 39)	(255 27)	(257 11)	(259 17)	(260 9)
(261 12)	(264 8)	(266 15)	(267 5)	(268 3)
(271 21)	(274 19)	(275 24)	(276 20)	(277 35)
(278 21)	(279 16)	(280 5)	(283 15)	(285 9)
(286 9)	(291 17)	(292 6)	(293 10)	(294 4)
(297 7)	(298 10)	(299 11)	(300 7)	(301 71)
(302 27)	(303 7)	(305 6)	(306 8)	(307 40)
(308 21)	(309 6)	(313 97)	(314 40)	(315 8)
(319 10)	(320 10)	(322 18)	(323 12)	(325 9)
(326 13)	(327 37)	(328 20)	(329 29)	(330 16)
(332 14)	(333 36)	(334 6)	(336 13)	(337 64)
(338 16)	(341 21)	(345 5)	(346 18)	(347 10)
(348 10)	(349 3)	(350 14)	(351 7)	(352 24)
(353 11)	(359 3)	(360 14)	(361 15)	(362 25)
(363 81)	(364 24)	(365 3)	(366 10)	(367 13)
(370 3)	(371 5)	(373 11)	(377 17)	(378 31)
(379 5)	(380 12)	(381 19)	(382 5)	(383 27)
(384 16)	(385 27)	(386 7)	(388 3)	(391 14)
(395 13)	(397 11)	(401 13)	(402 3)	(408 6)
(409 4)	(410 18)	(414 3)	(417 7)	(422 16)
(425 7)	(426 21)	(427 21)	(429 5)	(432 10)
(439 12)	(440 27)	(442 11)	(443 9)	(446 11)

199

(447	13)	(449	21)	(450	29)	(453	3)	(456	6)
(459	6)	(463	3)	(465	12)	(466	42)	(467	25)
(468	38)	(469	35)	(470	5)	(471	14)	(472	15)
(473	4)	(475	31)	(476	24)	(480	13)	(489	23)
(490	4)	(491	8)	(494	5)	(495	20)	(497	14)
(498	8)	(500	16)	(501	3)	(502	7)	(503	25)
(508	7)	(509	12)	(511	5)	(512	8)	(514	16)
(515	10)	(516	10)	(518	11)	(521	17)	(522	15)
(524	12)	(525	11)	(526	4)	(527	4)	(528	13)
(535	26)	(538	4)	(540	16)	(542	14)	(543	21)
(544	17)	(545	5)	(550	3)	(551	5)	(553	4)
(556	10)	(559	5)	(564	3)	(569	5)	(573	3)
(575	7)	(580	10)	(583	9)	(585	6)	(589	9)
(590	10)	(593	5)	(595	4)	(597	5)	(598	7)

NAME:12C\_3183.2\_1160EC23\_[748; D-Sedoheptulose-7-phosphate (7TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:318001-10-1

RI:3183

RT:19.137

NUM PEAKS: 111

( 72	7)	( 73	1000)	( 74	84)	( 81	30)	( 85	8)
( 87	4)	(101	10)	(103	105)	(104	6)	(109	15)
(113	17)	(116	8)	(117	37)	(118	5)	(127	6)
(129	140)	(130	16)	(131	26)	(132	7)	(133	54)
(134	7)	(135	6)	(141	4)	(142	8)	(143	24)
(145	8)	(147	322)	(148	49)	(149	36)	(151	3)
(153	7)	(155	28)	(156	4)	(157	15)	(169	46)
(170	8)	(171	9)	(173	6)	(175	4)	(181	3)
(183	10)	(189	26)	(191	38)	(199	4)	(203	7)
(204	42)	(205	20)	(206	6)	(208	14)	(209	9)
(211	33)	(212	4)	(213	4)	(217	93)	(218	21)
(219	10)	(225	5)	(227	14)	(228	4)	(231	9)
(233	5)	(242	23)	(243	45)	(244	13)	(245	10)
(253	4)	(255	4)	(257	4)	(269	3)	(270	22)
(271	200)	(272	50)	(273	21)	(291	7)	(293	3)
(294	3)	(298	6)	(299	80)	(300	22)	(301	11)
(302	4)	(305	7)	(314	10)	(315	225)	(316	65)
(317	34)	(318	8)	(319	7)	(341	11)	(343	6)
(357	11)	(358	5)	(360	3)	(361	32)	(362	12)
(363	6)	(372	4)	(386	10)	(387	78)	(388	33)
(389	18)	(422	3)	(423	23)	(424	5)	(431	3)
(454	3)	(484	3)	(512	6)	(513	32)	(514	20)
(515	10)								

NAME:12C\_2723.7\_1160EC23\_[777; Fructose-6-phosphate methoxyamine (6TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:272001-10-1

RI:2724

RT:17.023

NUM PEAKS: 75

( 73	1000)	( 74	78)	( 89	58)	( 90	7)	( 91	10)
(101	64)	(121	7)	(127	7)	(129	155)	(133	57)
(135	29)	(140	9)	(142	112)	(143	18)	(151	18)
(165	5)	(173	74)	(174	38)	(180	8)	(181	18)
(193	12)	(195	26)	(207	20)	(211	84)	(212	11)
(214	6)	(217	158)	(218	22)	(225	66)	(226	14)
(227	23)	(228	14)	(236	16)	(269	10)	(283	16)
(285	12)	(298	13)	(299	334)	(300	83)	(301	35)
(313	14)	(314	19)	(315	343)	(316	95)	(317	41)

200

(318	10)	(328	5)	(341	8)	(342	5)	(354	20)
(357	43)	(358	13)	(379	3)	(386	35)	(387	255)
(388	100)	(389	56)	(390	11)	(394	6)	(410	3)
(414	13)	(449	5)	(451	15)	(453	6)	(454	3)
(459	21)	(460	6)	(461	9)	(474	5)	(542	5)
(543	4)	(544	10)	(545	9)	(546	6)	(558	3)

NAME:12C\_2578.1\_1274EC11\_[734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:258001-10-1

RI:2578

RT:16.266

NUM PEAKS: 108

( 70	43)	( 71	35)	( 72	24)	( 73	1000)	( 74	89)
( 75	313)	( 76	15)	( 77	38)	( 79	66)	( 80	23)
( 81	185)	( 82	42)	( 83	124)	( 84	32)	( 85	27)
( 89	40)	( 91	22)	( 93	50)	( 94	18)	( 95	108)
( 96	33)	( 97	79)	( 98	48)	( 99	32)	(100	8)
(101	139)	(102	18)	(103	308)	(104	30)	(105	33)
(106	6)	(107	31)	(108	14)	(109	50)	(110	12)
(111	45)	(112	12)	(113	24)	(115	23)	(116	79)
(117	133)	(118	20)	(119	31)	(120	14)	(121	53)
(122	10)	(123	40)	(124	6)	(125	16)	(129	580)
(130	102)	(131	154)	(132	49)	(133	124)	(134	27)
(135	67)	(136	17)	(137	35)	(139	10)	(145	52)
(146	40)	(147	444)	(148	75)	(149	84)	(150	14)
(151	20)	(152	7)	(153	13)	(159	6)	(161	9)
(162	4)	(163	24)	(165	16)	(171	6)	(175	20)
(176	9)	(187	14)	(188	19)	(192	9)	(201	90)
(202	20)	(203	127)	(205	58)	(206	10)	(215	23)
(219	34)	(220	6)	(221	14)	(236	15)	(237	53)
(238	12)	(243	7)	(244	7)	(255	6)	(257	40)
(258	20)	(272	5)	(279	22)	(286	13)	(311	11)
(339	7)	(369	106)	(370	46)	(371	17)	(382	19)
(457	17)	(458	14)	(475	3)				

NAME:12C\_2386.9\_1160EC23\_[928; Glucopyranose-6-phosphate (6TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:239001-10-1

RI:2387

RT:15.242

NUM PEAKS: 78

( 72	12)	( 73	1000)	( 74	84)	( 75	100)	( 81	17)
( 87	3)	( 99	4)	(101	20)	(111	6)	(113	18)
(115	6)	(116	9)	(127	4)	(129	153)	(130	15)
(131	24)	(133	58)	(134	6)	(135	9)	(143	15)
(147	180)	(148	25)	(149	21)	(151	5)	(155	10)
(161	4)	(169	10)	(181	6)	(189	25)	(190	5)
(191	46)	(192	7)	(193	8)	(195	5)	(204	221)
(205	43)	(206	16)	(207	12)	(208	3)	(211	37)
(212	5)	(217	57)	(219	5)	(225	9)	(227	9)
(231	5)	(242	5)	(243	12)	(247	6)	(253	4)
(269	5)	(270	7)	(271	18)	(272	4)	(283	3)
(285	3)	(298	4)	(299	110)	(300	29)	(301	14)
(314	4)	(315	40)	(316	11)	(317	8)	(345	8)
(357	36)	(358	11)	(359	5)	(369	3)	(370	20)
(371	7)	(372	3)	(373	3)	(386	14)	(387	120)
(388	48)	(389	28)	(390	7)				

NAME:12C\_2310.0\_1191EC10\_Fructose-6-phosphate methoxyamine (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:232002-10-1

RI:2310

RT:14.783

NUM PEAKS: 127

( 70	8)	( 71	11)	( 72	15)	( 73	1000)	( 74	90)
( 75	89)	( 76	4)	( 77	8)	( 81	4)	( 82	3)
( 83	7)	( 84	28)	( 85	11)	( 87	4)	( 88	3)
( 89	47)	( 90	5)	( 91	4)	( 93	3)	( 95	3)
( 97	5)	( 98	4)	( 99	6)	(100	7)	(101	32)
(102	6)	(103	73)	(104	9)	(105	6)	(111	4)
(113	7)	(114	11)	(115	9)	(116	11)	(117	21)
(118	3)	(119	7)	(126	5)	(127	5)	(128	3)
(129	65)	(130	7)	(131	18)	(132	3)	(133	56)
(134	7)	(135	11)	(137	3)	(141	3)	(142	5)
(143	7)	(147	129)	(148	21)	(149	14)	(151	4)
(152	4)	(155	4)	(156	4)	(157	5)	(159	3)
(163	5)	(169	4)	(172	5)	(173	5)	(180	3)
(181	6)	(182	4)	(183	3)	(189	7)	(190	3)
(191	11)	(193	6)	(195	7)	(196	3)	(197	3)
(204	10)	(205	8)	(206	3)	(207	11)	(208	3)
(209	4)	(211	29)	(212	6)	(213	3)	(214	3)
(217	81)	(218	19)	(219	7)	(221	5)	(225	11)
(226	3)	(227	8)	(232	4)	(243	5)	(244	4)
(245	4)	(260	3)	(270	3)	(271	3)	(283	3)
(285	5)	(286	3)	(298	5)	(299	64)	(300	23)
(301	11)	(302	4)	(313	3)	(314	8)	(315	105)
(316	31)	(317	15)	(318	5)	(319	3)	(341	5)
(342	3)	(355	3)	(356	4)	(357	15)	(358	5)
(359	3)	(373	3)	(403	5)	(458	3)	(459	9)
(460	4)	(461	3)						

NAME:12C\_2257.2\_1160EC23\_[715; Erythritol (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:226001-10-1

RI:2257

RT:14.556

NUM PEAKS: 143

( 70	24)	( 72	14)	( 73	1000)	( 74	61)	( 75	94)
( 76	5)	( 80	4)	( 82	13)	( 83	9)	( 84	290)
( 85	22)	( 86	22)	( 88	3)	( 89	36)	( 90	3)
( 94	4)	( 96	3)	( 99	8)	(100	17)	(101	8)
(102	8)	(103	227)	(104	20)	(105	11)	(108	3)
(111	12)	(112	3)	(113	7)	(114	8)	(115	4)
(116	24)	(117	66)	(118	8)	(119	6)	(123	3)
(126	3)	(127	3)	(128	11)	(129	34)	(130	10)
(131	18)	(132	6)	(133	45)	(134	5)	(135	6)
(140	4)	(141	6)	(142	33)	(143	20)	(144	43)
(145	9)	(146	4)	(147	210)	(148	32)	(149	20)
(153	3)	(154	3)	(155	4)	(157	12)	(158	11)
(159	4)	(161	3)	(163	4)	(167	4)	(168	6)
(169	3)	(170	7)	(171	4)	(172	14)	(173	15)
(174	53)	(175	11)	(176	3)	(180	3)	(182	4)
(183	8)	(184	3)	(186	11)	(187	5)	(188	5)
(189	18)	(190	3)	(191	9)	(198	3)	(200	7)
(201	8)	(202	30)	(203	6)	(204	13)	(205	31)
(206	7)	(207	3)	(213	6)	(214	5)	(216	3)
(217	93)	(218	20)	(219	7)	(221	4)	(225	12)
(226	3)	(232	3)	(242	5)	(243	3)	(244	4)

202

(256	5)	(257	9)	(258	4)	(260	3)	(268	4)
(269	3)	(270	4)	(271	5)	(277	6)	(300	3)
(307	9)	(308	3)	(316	3)	(330	12)	(331	8)
(332	3)	(342	5)	(343	4)	(367	4)	(372	3)
(373	34)	(374	19)	(375	8)	(376	3)	(403	4)
(404	3)	(437	4)	(447	9)	(448	6)	(457	4)
(476	3)	(477	3)	(547	7)	(548	6)	(550	3)
(551	7)	(552	6)	(553	3)				

NAME: 12C\_2718.4\_1313EC43\_[824; D-Sedoheptulose-7-phosphate (7TMS)]

COMMENTS: Kopka J, MPIMP, Dept. Willmitzer

CASNO: 272002-10-1

RI: 2718

RT: 16.521

NUM PEAKS: 469

( 70	2)	( 72	15)	( 73	1000)	( 74	86)	( 75	58)
( 76	3)	( 77	6)	( 79	1)	( 80	1)	( 81	6)
( 82	6)	( 84	2)	( 86	3)	( 87	6)	( 88	3)
( 89	24)	( 90	3)	( 91	3)	( 92	2)	( 93	3)
( 94	2)	( 95	1)	( 96	2)	( 98	4)	(100	6)
(101	39)	(102	6)	(103	47)	(104	6)	(105	10)
(106	3)	(107	7)	(108	2)	(109	4)	(110	1)
(111	4)	(112	2)	(113	7)	(114	6)	(115	11)
(116	18)	(117	22)	(118	3)	(119	8)	(120	2)
(121	6)	(122	3)	(123	3)	(124	3)	(125	1)
(126	3)	(127	3)	(128	4)	(129	113)	(130	16)
(131	22)	(132	7)	(133	62)	(134	9)	(135	18)
(136	4)	(137	11)	(138	4)	(139	3)	(140	4)
(141	1)	(142	25)	(143	12)	(144	3)	(145	7)
(146	2)	(147	132)	(148	23)	(149	16)	(150	3)
(151	9)	(152	3)	(153	4)	(154	4)	(155	8)
(156	5)	(157	10)	(158	5)	(159	4)	(160	12)
(161	10)	(162	2)	(163	7)	(164	2)	(165	4)
(166	4)	(167	4)	(168	5)	(169	13)	(170	6)
(171	6)	(172	4)	(173	25)	(174	5)	(175	5)
(176	2)	(177	2)	(178	2)	(179	4)	(180	7)
(181	12)	(182	6)	(183	7)	(184	3)	(185	3)
(186	3)	(187	2)	(188	2)	(189	16)	(190	6)
(191	104)	(192	18)	(193	19)	(194	4)	(195	12)
(196	8)	(197	5)	(198	4)	(199	8)	(200	4)
(201	2)	(202	2)	(203	5)	(204	103)	(205	19)
(206	7)	(207	18)	(208	5)	(209	7)	(210	5)
(211	58)	(212	10)	(213	7)	(214	2)	(215	4)
(216	4)	(217	121)	(218	31)	(219	15)	(220	2)
(221	3)	(222	1)	(223	1)	(224	2)	(225	25)
(226	6)	(227	16)	(228	7)	(229	4)	(230	4)
(231	6)	(232	2)	(233	2)	(234	2)	(235	1)
(236	8)	(237	2)	(238	1)	(239	1)	(240	3)
(241	5)	(242	4)	(243	16)	(244	3)	(245	3)
(246	1)	(247	4)	(248	1)	(249	1)	(250	2)
(251	2)	(252	2)	(253	4)	(254	4)	(255	4)
(256	2)	(257	3)	(258	2)	(259	4)	(260	2)
(261	3)	(262	1)	(263	1)	(264	2)	(265	2)
(266	3)	(267	3)	(268	5)	(269	5)	(270	5)
(271	5)	(272	4)	(273	2)	(274	2)	(275	2)
(276	1)	(277	3)	(278	2)	(279	2)	(280	1)
(281	1)	(282	3)	(283	7)	(284	4)	(285	8)
(286	4)	(287	2)	(289	4)	(290	2)	(291	3)
(292	3)	(294	1)	(295	1)	(297	2)	(298	12)
(299	132)	(300	41)	(301	20)	(302	3)	(303	2)



(304	4)	(305	6)	(306	4)	(307	3)	(308	2)
(309	2)	(310	1)	(311	2)	(312	2)	(313	4)
(314	14)	(315	128)	(316	36)	(317	20)	(318	5)
(320	1)	(322	2)	(323	1)	(325	1)	(326	1)
(327	2)	(328	2)	(329	3)	(330	3)	(331	2)
(332	2)	(335	2)	(337	1)	(339	2)	(340	2)
(341	6)	(342	2)	(343	2)	(345	3)	(346	2)
(347	1)	(348	3)	(349	2)	(350	1)	(351	1)
(352	3)	(353	4)	(354	12)	(355	5)	(356	7)
(357	21)	(358	8)	(359	4)	(360	5)	(361	29)
(362	9)	(363	6)	(364	4)	(365	3)	(366	1)
(367	2)	(368	2)	(369	1)	(370	3)	(371	3)
(372	2)	(373	4)	(374	2)	(375	2)	(376	2)
(377	1)	(380	1)	(381	2)	(382	2)	(383	1)
(384	2)	(385	3)	(386	20)	(387	81)	(388	32)
(389	15)	(390	4)	(391	1)	(392	2)	(393	2)
(394	1)	(395	2)	(396	3)	(397	1)	(398	2)
(399	1)	(400	1)	(401	2)	(402	1)	(403	2)
(404	2)	(405	1)	(406	1)	(408	1)	(409	1)
(410	2)	(411	2)	(413	4)	(414	11)	(415	4)
(416	4)	(417	2)	(418	3)	(419	1)	(420	1)
(421	1)	(422	1)	(423	2)	(424	2)	(425	1)
(426	1)	(427	1)	(428	1)	(429	1)	(430	2)
(431	1)	(432	2)	(433	2)	(434	3)	(435	1)
(436	3)	(437	4)	(438	3)	(439	1)	(440	1)
(441	1)	(442	3)	(443	2)	(444	1)	(445	1)
(446	1)	(448	2)	(449	2)	(450	4)	(451	5)
(452	4)	(453	3)	(454	3)	(455	1)	(456	1)
(457	1)	(458	4)	(459	12)	(460	6)	(461	3)
(462	1)	(463	2)	(466	1)	(467	1)	(468	1)
(469	1)	(470	2)	(471	1)	(472	2)	(473	1)
(475	1)	(476	2)	(480	2)	(481	2)	(482	1)
(483	1)	(484	2)	(485	1)	(486	3)	(487	2)
(489	2)	(490	1)	(491	2)	(492	2)	(493	1)
(494	1)	(495	2)	(496	1)	(498	2)	(499	2)
(500	2)	(502	2)	(503	2)	(504	1)	(505	1)
(506	2)	(507	1)	(508	2)	(509	2)	(511	2)
(512	2)	(513	1)	(514	1)	(515	1)	(516	2)
(517	1)	(518	2)	(519	2)	(521	1)	(522	3)
(523	2)	(524	1)	(525	3)	(526	2)	(527	3)
(530	2)	(531	1)	(533	1)	(534	3)	(535	1)
(536	1)	(537	1)	(538	3)	(539	2)	(540	2)
(541	2)	(542	2)	(543	1)	(544	2)	(545	3)
(546	2)	(547	1)	(548	2)	(549	1)	(550	1)
(551	1)	(553	1)	(554	1)	(555	1)	(556	2)
(557	1)	(558	1)	(559	1)	(560	1)	(561	1)
(562	1)	(563	1)	(564	1)	(565	1)	(566	1)
(571	1)	(572	1)	(573	1)	(574	1)	(575	1)
(577	1)	(578	1)	(581	1)	(588	1)		

NAME:12C\_2347.2\_1313EC43\_Glucose-6-phosphate methoxyamine (BP) (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:235002-10-1

RI:2347

RT: 14.555

NUM PEAKS: 146

( 72	15)	( 73	1000)	( 74	81)	( 75	103)	( 76	7)
( 77	11)	( 79	7)	( 80	3)	( 81	6)	( 86	4)
( 87	4)	( 88	3)	( 89	46)	( 90	5)	( 91	8)
( 92	2)	( 93	3)	( 95	4)	( 97	3)	( 98	3)

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(100	8)	(101	37)	(102	9)	(103	48)	(104	4)
(105	14)	(106	5)	(107	3)	(108	2)	(109	2)
(114	8)	(115	11)	(116	19)	(118	2)	(119	8)
(121	3)	(129	69)	(130	16)	(131	30)	(133	66)
(134	10)	(135	14)	(136	2)	(137	4)	(138	2)
(142	2)	(143	11)	(144	2)	(145	7)	(146	2)
(147	132)	(148	19)	(149	18)	(150	4)	(151	5)
(154	2)	(157	32)	(158	4)	(159	6)	(160	38)
(161	13)	(162	2)	(163	5)	(172	2)	(173	3)
(174	2)	(175	2)	(176	2)	(177	2)	(180	2)
(181	6)	(188	1)	(189	8)	(190	1)	(191	14)
(192	3)	(193	8)	(194	2)	(195	4)	(197	2)
(201	3)	(203	5)	(204	7)	(205	8)	(207	16)
(211	38)	(212	6)	(213	5)	(215	2)	(216	3)
(217	30)	(218	6)	(225	10)	(226	2)	(227	8)
(228	5)	(229	4)	(230	3)	(231	2)	(241	3)
(243	5)	(244	3)	(245	2)	(247	8)	(253	3)
(265	1)	(268	2)	(269	5)	(270	1)	(278	1)
(283	3)	(285	4)	(298	8)	(299	92)	(300	26)
(301	11)	(314	9)	(315	43)	(316	12)	(317	6)
(318	1)	(319	2)	(331	4)	(332	2)	(341	4)
(356	6)	(357	27)	(358	8)	(359	3)	(370	2)
(373	3)	(374	2)	(385	2)	(386	27)	(387	101)
(388	39)	(389	19)	(390	3)	(409	1)	(435	1)
(470	4)	(471	9)	(472	3)	(473	3)	(501	2)
(569	1)								

NAME:12C\_2039.0\_1313EC43\_[607; Putrescine (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:204003-10-1

RI:2039

RT: 12.763

NUM PEAKS: 219

( 70	80)	( 71	135)	( 72	41)	( 73	616)	( 74	121)
( 75	287)	( 76	2)	( 79	19)	( 80	11)	( 81	17)
( 82	3)	( 83	22)	( 84	132)	( 85	103)	( 86	256)
( 87	53)	( 88	26)	( 93	10)	( 94	4)	( 95	7)
( 96	3)	( 98	29)	( 99	150)	(100	259)	(101	1)
(102	49)	(108	1)	(110	49)	(111	4)	(112	71)
(113	21)	(114	42)	(115	4)	(116	31)	(122	9)
(123	11)	(124	12)	(125	2)	(126	152)	(127	44)
(128	7)	(130	106)	(131	25)	(140	26)	(141	9)
(142	128)	(143	10)	(146	57)	(147	116)	(148	31)
(150	4)	(152	9)	(153	7)	(154	21)	(155	10)
(156	5)	(157	5)	(158	12)	(160	252)	(161	1)
(162	7)	(164	5)	(166	9)	(167	14)	(168	5)
(169	1)	(170	3)	(172	112)	(173	4)	(174	407)
(175	51)	(176	45)	(179	18)	(180	6)	(181	13)
(182	4)	(183	5)	(185	2)	(186	34)	(188	24)
(194	5)	(197	7)	(198	9)	(200	118)	(201	19)
(204	129)	(207	10)	(208	9)	(210	3)	(212	6)
(213	5)	(214	1000)	(215	205)	(216	97)	(231	9)
(232	4)	(233	3)	(239	9)	(240	12)	(241	4)
(242	1)	(245	3)	(246	28)	(250	6)	(251	3)
(252	12)	(253	1)	(257	3)	(258	13)	(259	2)
(261	5)	(266	11)	(267	5)	(268	27)	(269	18)
(270	5)	(272	3)	(276	1)	(280	7)	(281	1)
(282	3)	(283	12)	(287	5)	(288	49)	(289	13)
(291	11)	(292	21)	(295	3)	(305	1)	(311	17)
(319	30)	(320	4)	(321	6)	(324	2)	(325	5)

## 205

(330	9)	(331	2)	(332	2)	(334	4)	(336	7)
(339	17)	(352	9)	(353	2)	(355	15)	(356	10)
(358	1)	(360	1)	(361	6)	(363	2)	(367	1)
(372	14)	(374	8)	(375	61)	(376	48)	(377	18)
(381	3)	(395	14)	(398	2)	(407	2)	(412	2)
(416	2)	(420	2)	(425	8)	(430	3)	(435	1)
(439	2)	(443	1)	(444	3)	(448	8)	(452	4)
(454	2)	(455	2)	(456	6)	(457	9)	(458	6)
(461	4)	(462	8)	(465	4)	(467	7)	(469	3)
(471	4)	(474	12)	(475	21)	(476	9)	(478	13)
(479	5)	(482	4)	(483	6)	(484	6)	(488	5)
(489	3)	(493	15)	(494	2)	(497	15)	(501	10)
(502	2)	(504	1)	(505	4)	(506	2)	(513	7)
(525	2)	(526	3)	(527	7)	(530	7)	(538	1)
(547	2)	(550	4)	(552	7)	(563	3)	(566	1)
(571	2)	(575	11)	(580	5)	(583	6)	(586	5)
(589	2)	(590	1)	(592	6)	(595	4)		

NAME:12C\_1476.2\_1313EC75\_Citramalic acid (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:148001-10-1

RI:1476

RT: 8.471

NUM PEAKS: 38

( 73	1000)	( 74	89)	( 75	222)	( 76	14)	( 85	40)
( 86	6)	(115	117)	(116	15)	(117	41)	(131	33)
(133	83)	(134	10)	(143	17)	(144	8)	(147	404)
(148	65)	(149	70)	(150	8)	(151	5)	(157	14)
(163	29)	(164	5)	(185	18)	(190	8)	(203	33)
(205	6)	(219	3)	(221	14)	(231	32)	(233	26)
(247	141)	(248	31)	(259	33)	(260	7)	(261	4)
(321	16)	(322	6)	(349	10)				

NAME:12C\_1735.8\_1313EC75\_Glycerol-2-phosphate (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:174002-10-1

RI:1736

RT: 10.585

NUM PEAKS: 393

( 70	9)	( 71	14)	( 72	24)	( 73	1000)	( 74	81)
( 75	224)	( 76	10)	( 77	18)	( 78	7)	( 79	14)
( 80	4)	( 81	5)	( 82	4)	( 83	5)	( 84	16)
( 85	11)	( 86	7)	( 87	13)	( 88	4)	( 89	25)
( 90	4)	( 91	8)	( 92	6)	( 93	7)	( 94	5)
( 95	5)	( 96	5)	( 97	9)	( 98	6)	( 99	10)
(100	10)	(101	93)	(102	12)	(103	111)	(104	10)
(105	15)	(106	9)	(107	4)	(108	1)	(109	3)
(110	4)	(111	6)	(112	2)	(113	11)	(114	6)
(115	21)	(116	55)	(117	43)	(118	11)	(119	9)
(120	3)	(121	6)	(122	2)	(123	7)	(124	3)
(125	1)	(126	2)	(127	6)	(128	3)	(129	114)
(130	15)	(131	43)	(132	5)	(133	84)	(134	16)
(135	15)	(136	3)	(137	9)	(138	5)	(139	4)
(140	5)	(141	11)	(142	8)	(143	10)	(144	2)
(145	1)	(146	4)	(147	224)	(148	39)	(149	30)
(150	5)	(151	7)	(152	4)	(153	56)	(154	9)
(155	8)	(156	1)	(157	10)	(159	27)	(160	9)
(161	4)	(162	1)	(163	8)	(166	3)	(167	12)
(168	5)	(169	10)	(170	8)	(171	5)	(174	7)
(175	5)	(176	3)	(177	8)	(178	1)	(179	3)

(180	6)	(181	10)	(182	3)	(183	6)	(184	1)
(185	3)	(186	3)	(187	5)	(188	4)	(189	16)
(190	6)	(191	17)	(192	7)	(193	14)	(194	6)
(195	9)	(196	1)	(197	4)	(198	1)	(199	1)
(200	3)	(201	1)	(203	6)	(204	33)	(205	23)
(206	3)	(207	24)	(210	3)	(211	90)	(212	20)
(213	10)	(214	1)	(215	4)	(216	1)	(217	61)
(218	20)	(219	8)	(220	4)	(221	2)	(222	3)
(223	2)	(225	6)	(226	4)	(227	20)	(228	5)
(229	5)	(230	3)	(231	16)	(232	8)	(233	3)
(234	3)	(235	4)	(236	1)	(237	5)	(239	5)
(240	2)	(241	25)	(242	7)	(243	129)	(244	18)
(245	7)	(246	2)	(247	3)	(248	4)	(249	2)
(250	3)	(253	3)	(254	3)	(257	1)	(258	2)
(259	2)	(260	1)	(261	2)	(263	2)	(264	2)
(265	2)	(266	2)	(267	2)	(268	5)	(269	9)
(270	6)	(271	5)	(272	1)	(273	2)	(274	4)
(275	4)	(277	4)	(279	1)	(280	2)	(281	2)
(283	3)	(284	11)	(285	16)	(286	4)	(287	6)
(293	1)	(294	6)	(297	1)	(298	11)	(299	63)
(300	22)	(301	11)	(302	5)	(304	5)	(305	16)
(306	13)	(307	10)	(308	5)	(309	4)	(310	1)
(311	1)	(313	3)	(314	3)	(315	13)	(316	5)
(317	2)	(318	3)	(319	9)	(320	4)	(321	4)
(322	1)	(323	4)	(324	1)	(325	1)	(326	3)
(327	3)	(328	4)	(331	2)	(332	2)	(338	5)
(339	1)	(340	2)	(341	2)	(342	6)	(343	3)
(345	3)	(346	1)	(349	2)	(350	1)	(352	3)
(353	2)	(355	3)	(357	3)	(358	4)	(359	3)
(360	1)	(361	3)	(365	1)	(367	1)	(368	1)
(369	3)	(372	1)	(373	5)	(374	2)	(375	4)
(376	4)	(377	4)	(378	3)	(379	2)	(380	1)
(381	1)	(382	2)	(383	2)	(384	1)	(385	4)
(386	3)	(387	4)	(388	1)	(389	10)	(390	8)
(391	4)	(393	3)	(395	1)	(396	2)	(397	2)
(398	1)	(399	3)	(400	2)	(401	2)	(404	3)
(405	2)	(406	2)	(407	2)	(411	2)	(412	2)
(415	4)	(416	3)	(417	1)	(421	1)	(422	3)
(423	1)	(424	2)	(427	4)	(428	3)	(430	1)
(432	2)	(434	1)	(438	4)	(439	2)	(444	4)
(445	7)	(446	2)	(448	4)	(449	4)	(450	2)
(452	3)	(453	4)	(454	2)	(457	2)	(458	4)
(460	1)	(461	2)	(462	1)	(463	1)	(464	4)
(465	2)	(466	2)	(467	4)	(468	3)	(469	3)
(472	4)	(473	3)	(476	3)	(477	3)	(480	2)
(481	2)	(482	3)	(486	2)	(487	1)	(488	2)
(491	1)	(492	2)	(493	2)	(494	7)	(495	2)
(497	5)	(498	2)	(500	1)	(502	4)	(503	5)
(504	5)	(505	1)	(506	2)	(507	1)	(510	3)
(511	4)	(514	4)	(515	1)	(517	5)	(518	3)
(519	3)	(521	1)	(522	4)	(523	2)	(524	3)
(526	4)	(527	2)	(529	1)	(530	1)	(534	6)
(537	2)	(538	2)	(541	2)	(543	2)	(544	4)
(545	1)	(547	1)	(548	5)	(552	4)	(554	3)
(555	4)	(556	1)	(561	1)	(562	1)	(563	1)
(564	3)	(565	1)	(566	4)	(567	3)	(570	1)
(572	1)	(574	1)	(575	1)	(579	1)	(582	1)
(583	3)	(596	1)	(597	1)				

NAME:12C\_1761.3\_1313EC75\_[757; 2-Desoxy-pentos-3-ylose dimethoxyamine  
(2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:176004-10-1

RI:1762

RT: 10.782

NUM PEAKS: 86

( 73	1000)	( 74	100)	( 81	5)	( 89	133)	( 93	3)
( 94	5)	( 95	18)	(101	53)	(103	122)	(104	11)
(105	57)	(106	6)	(107	3)	(108	5)	(111	10)
(117	87)	(118	10)	(119	17)	(121	9)	(123	3)
(126	14)	(133	157)	(134	19)	(135	12)	(136	1)
(137	3)	(142	278)	(143	52)	(147	234)	(148	41)
(149	31)	(153	8)	(163	16)	(164	3)	(167	17)
(179	1)	(180	3)	(181	5)	(189	12)	(190	5)
(191	17)	(192	3)	(194	2)	(195	4)	(197	3)
(198	2)	(199	25)	(201	27)	(202	3)	(204	12)
(205	51)	(206	9)	(207	3)	(209	1)	(212	3)
(217	50)	(218	9)	(219	3)	(225	8)	(226	4)
(230	7)	(231	667)	(232	103)	(233	28)	(234	3)
(241	2)	(256	1)	(257	10)	(271	3)	(273	5)
(277	2)	(307	7)	(314	3)	(315	27)	(316	7)
(331	5)	(332	3)	(333	5)	(334	2)	(346	2)
(373	1)	(404	1)	(405	9)	(406	3)	(407	2)
(421	3)								

NAME:12C\_1796.4\_1313EC75\_[646; 3-Deoxyglucitol (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:180001-10-1

RI:1796

RT: 11.055

NUM PEAKS: 263

( 70	11)	( 71	11)	( 72	24)	( 73	1000)	( 74	90)
( 75	119)	( 76	9)	( 77	4)	( 79	1)	( 80	4)
( 81	5)	( 82	6)	( 83	2)	( 84	42)	( 85	18)
( 87	7)	( 88	5)	( 89	70)	( 90	7)	( 91	6)
( 92	1)	( 93	8)	( 94	4)	( 95	110)	( 96	10)
( 97	4)	( 98	14)	( 99	11)	(100	10)	(101	45)
(102	7)	(103	123)	(104	12)	(105	92)	(106	9)
(107	5)	(108	3)	(109	2)	(110	3)	(111	11)
(112	7)	(113	6)	(114	1)	(115	9)	(116	22)
(117	67)	(118	9)	(119	11)	(120	2)	(121	7)
(122	3)	(123	10)	(125	3)	(126	21)	(127	8)
(128	3)	(129	26)	(130	7)	(131	28)	(132	6)
(133	77)	(134	9)	(135	8)	(136	3)	(137	2)
(138	3)	(139	7)	(140	4)	(141	4)	(142	21)
(143	14)	(144	4)	(145	4)	(146	3)	(147	192)
(148	29)	(149	26)	(150	3)	(151	4)	(152	3)
(153	8)	(155	4)	(156	15)	(157	7)	(158	17)
(159	6)	(160	2)	(161	2)	(162	1)	(163	8)
(164	2)	(165	2)	(166	2)	(167	22)	(168	7)
(169	5)	(170	4)	(172	2)	(173	3)	(175	4)
(177	2)	(179	2)	(180	1)	(181	3)	(182	2)
(183	6)	(184	4)	(185	3)	(186	7)	(187	3)
(189	10)	(191	20)	(192	3)	(193	2)	(194	3)
(195	4)	(196	2)	(198	2)	(199	90)	(200	17)
(201	29)	(202	6)	(203	2)	(204	10)	(205	44)
(206	8)	(209	2)	(210	1)	(211	2)	(212	5)
(213	3)	(214	2)	(215	2)	(216	11)	(217	55)
(218	11)	(219	5)	(221	1)	(223	1)	(225	7)

208

(226	2)	(227	2)	(228	5)	(229	2)	(230	5)
(231	105)	(232	17)	(233	5)	(235	1)	(236	1)
(241	1)	(242	2)	(243	9)	(244	2)	(245	1)
(248	1)	(249	1)	(253	1)	(254	1)	(255	2)
(256	2)	(257	7)	(261	1)	(266	1)	(268	1)
(269	3)	(270	2)	(271	2)	(273	5)	(274	2)
(275	1)	(277	3)	(278	2)	(285	2)	(287	1)
(288	1)	(289	1)	(290	1)	(291	1)	(296	1)
(299	2)	(300	2)	(302	2)	(304	1)	(305	1)
(306	2)	(307	12)	(308	4)	(309	2)	(314	2)
(315	21)	(316	6)	(317	2)	(318	3)	(319	1)
(323	1)	(327	1)	(329	1)	(330	1)	(331	4)
(332	2)	(333	6)	(334	2)	(335	1)	(336	1)
(337	1)	(342	1)	(344	1)	(346	2)	(347	1)
(351	2)	(352	1)	(358	1)	(359	1)	(361	1)
(365	1)	(367	1)	(376	1)	(381	1)	(399	1)
(402	1)	(404	2)	(405	5)	(406	2)	(412	1)
(414	1)	(420	1)	(421	2)	(422	1)	(424	1)
(425	1)	(428	1)	(432	1)	(439	1)	(455	1)
(456	1)	(462	1)	(465	1)	(475	1)	(479	1)
(480	1)	(495	1)	(502	1)	(504	1)	(510	1)
(516	1)	(517	1)	(520	1)	(523	1)	(524	1)
(528	1)	(529	2)	(531	1)	(542	1)	(543	1)
(545	1)	(547	1)	(548	1)	(552	1)	(560	1)
(566	1)	(571	1)	(590	1)				

NAME:12C\_3380.0\_1274EC11\_Lanosta-8,24-dien-3-beta-ol (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:338001-10-1

RI:3380

RT:19.985

NUM PEAKS: 215

( 70	99)	( 72	17)	( 73	1000)	( 74	97)	( 75	732)
( 76	67)	( 77	169)	( 78	49)	( 79	252)	( 80	28)
( 81	444)	( 82	57)	( 83	204)	( 84	20)	( 87	11)
( 88	10)	( 89	30)	( 90	10)	( 91	261)	( 92	37)
( 93	280)	( 94	37)	( 95	457)	( 96	40)	( 97	66)
( 98	10)	(101	17)	(103	35)	(104	10)	(105	295)
(106	41)	(107	273)	(108	41)	(109	538)	(110	48)
(111	54)	(114	8)	(115	59)	(116	25)	(117	129)
(118	27)	(119	293)	(120	52)	(121	251)	(122	49)
(123	179)	(124	19)	(125	12)	(127	19)	(128	54)
(129	244)	(130	55)	(131	184)	(132	37)	(133	211)
(134	47)	(135	237)	(136	39)	(137	88)	(138	15)
(139	7)	(141	38)	(142	39)	(143	124)	(144	40)
(145	191)	(146	42)	(147	212)	(148	45)	(149	134)
(150	22)	(151	31)	(152	15)	(153	14)	(154	16)
(155	38)	(156	26)	(157	133)	(158	38)	(159	167)
(160	64)	(161	167)	(162	37)	(163	80)	(164	15)
(165	29)	(166	14)	(167	13)	(168	10)	(169	36)
(170	17)	(171	89)	(172	33)	(173	129)	(174	42)
(175	117)	(176	18)	(177	45)	(178	11)	(179	16)
(181	12)	(182	8)	(183	36)	(184	16)	(185	72)
(186	24)	(187	158)	(188	33)	(189	139)	(190	34)
(191	69)	(192	17)	(193	20)	(197	27)	(198	13)
(199	59)	(200	21)	(201	71)	(202	21)	(203	55)
(204	20)	(205	18)	(206	8)	(207	64)	(208	12)
(209	11)	(211	27)	(212	15)	(213	52)	(214	29)
(215	86)	(216	21)	(217	31)	(219	10)	(220	7)
(225	28)	(226	11)	(227	79)	(228	20)	(229	79)

209

(230	18)	(231	14)	(232	4)	(233	6)	(237	6)
(239	14)	(240	8)	(241	136)	(242	33)	(243	36)
(244	12)	(245	10)	(253	15)	(254	8)	(255	57)
(256	17)	(257	34)	(258	11)	(259	9)	(265	10)
(266	9)	(267	18)	(269	25)	(270	12)	(271	17)
(272	22)	(273	11)	(281	29)	(282	11)	(283	27)
(284	7)	(285	11)	(286	5)	(295	9)	(297	16)
(298	8)	(299	6)	(309	15)	(310	6)	(311	27)
(312	11)	(317	5)	(319	6)	(323	15)	(325	10)
(328	6)	(331	9)	(332	6)	(335	4)	(349	5)
(350	11)	(351	15)	(352	9)	(386	8)	(389	3)
(393	276)	(394	162)	(395	38)	(408	4)	(413	10)
(427	4)	(450	6)	(477	4)	(482	11)	(483	70)
(484	72)	(485	27)	(486	9)	(487	5)	(497	14)
(498	77)	(499	67)	(500	28)	(501	10)	(506	6)

NAME:12C\_3081.9\_1160EC23\_[808; Adenosine-5'-monophosphate (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:308001-10-1

RI:3082

RT:18.685

NUM PEAKS: 174

( 70	5)	( 71	5)	( 72	18)	( 73	1000)	( 74	93)
( 75	110)	( 76	7)	( 77	11)	( 80	3)	( 81	29)
( 82	3)	( 85	8)	( 86	4)	( 87	5)	( 89	7)
( 92	3)	( 93	3)	( 94	5)	( 95	7)	( 97	12)
( 98	4)	( 99	14)	(100	3)	(101	27)	(102	6)
(103	12)	(105	4)	(107	3)	(108	29)	(109	5)
(111	8)	(113	18)	(114	3)	(115	18)	(116	11)
(117	11)	(118	3)	(119	14)	(120	3)	(121	6)
(125	9)	(126	3)	(127	11)	(129	66)	(130	9)
(131	20)	(132	5)	(133	78)	(134	12)	(135	85)
(136	80)	(137	12)	(139	3)	(140	24)	(141	15)
(142	18)	(143	26)	(144	4)	(145	7)	(146	3)
(147	143)	(148	30)	(149	24)	(150	6)	(151	9)
(153	12)	(154	3)	(155	5)	(156	3)	(157	6)
(158	3)	(159	4)	(160	3)	(161	4)	(162	3)
(163	3)	(164	40)	(165	8)	(167	6)	(168	3)
(169	469)	(170	67)	(171	44)	(172	6)	(173	4)
(174	4)	(175	4)	(177	3)	(178	3)	(179	4)
(181	12)	(183	6)	(184	5)	(185	4)	(186	7)
(187	3)	(189	4)	(190	3)	(191	6)	(193	10)
(194	5)	(195	14)	(196	3)	(197	5)	(204	3)
(205	3)	(206	20)	(207	27)	(208	31)	(209	8)
(210	4)	(211	83)	(212	13)	(213	8)	(214	10)
(215	16)	(216	5)	(217	18)	(218	5)	(221	3)
(225	18)	(226	3)	(227	17)	(228	4)	(229	4)
(230	125)	(231	29)	(232	12)	(233	3)	(234	16)
(235	4)	(241	3)	(243	67)	(244	15)	(245	9)
(248	3)	(249	4)	(250	16)	(251	3)	(253	4)
(257	6)	(258	69)	(259	20)	(260	8)	(262	7)
(265	22)	(266	7)	(283	3)	(285	7)	(298	3)
(299	74)	(300	23)	(301	12)	(302	5)	(303	6)
(304	13)	(305	3)	(306	8)	(307	3)	(314	8)
(315	240)	(316	64)	(317	33)	(318	6)	(371	9)
(372	3)	(382	21)	(383	9)	(384	4)	(387	4)
(394	20)	(395	8)	(396	3)	(411	3)		

NAME:12C\_2679.2\_1160EC23\_[837; alpha-D-Fructofuranose-1,6-bisphosphate (7TMS)]

210

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:268001-10-1

RI:2679

RT:16.787

NUM PEAKS: 170

( 71	4)	( 72	15)	( 73	1000)	( 74	88)	( 75	110)
( 76	6)	( 77	9)	( 81	8)	( 82	21)	( 83	7)
( 85	5)	( 86	3)	( 87	4)	( 89	5)	( 96	13)
( 97	7)	( 98	4)	( 99	6)	(100	3)	(101	15)
(102	6)	(103	33)	(104	4)	(105	3)	(109	8)
(111	5)	(113	12)	(115	8)	(116	5)	(117	21)
(118	3)	(119	6)	(125	5)	(127	6)	(128	3)
(129	86)	(130	14)	(131	20)	(133	53)	(134	7)
(135	13)	(137	4)	(140	13)	(141	17)	(142	11)
(143	24)	(144	6)	(145	5)	(146	3)	(147	199)
(148	32)	(149	29)	(150	3)	(151	9)	(153	3)
(155	9)	(156	8)	(157	17)	(158	4)	(159	3)
(163	3)	(167	3)	(169	12)	(177	9)	(181	7)
(182	3)	(183	11)	(184	4)	(187	3)	(189	10)
(190	7)	(191	37)	(192	6)	(193	10)	(195	10)
(196	5)	(197	4)	(199	3)	(200	14)	(201	4)
(202	3)	(203	3)	(204	37)	(205	17)	(206	5)
(207	25)	(208	5)	(209	5)	(210	3)	(211	49)
(212	8)	(213	6)	(214	11)	(215	57)	(216	14)
(217	63)	(218	14)	(219	8)	(221	33)	(222	9)
(223	5)	(225	29)	(226	6)	(227	16)	(228	3)
(229	9)	(230	68)	(231	23)	(232	7)	(241	6)
(243	10)	(244	3)	(255	5)	(257	36)	(258	9)
(259	5)	(269	3)	(270	4)	(271	15)	(272	4)
(273	3)	(281	7)	(283	8)	(284	3)	(285	9)
(295	10)	(296	3)	(297	3)	(298	7)	(299	124)
(300	34)	(301	18)	(302	3)	(303	7)	(305	3)
(313	5)	(314	7)	(315	166)	(316	46)	(317	24)
(318	5)	(319	7)	(328	22)	(329	7)	(330	3)
(341	3)	(343	6)	(345	4)	(347	6)	(348	3)
(355	3)	(356	4)	(357	10)	(358	3)	(361	3)
(369	7)	(370	3)	(371	3)	(373	7)	(387	17)
(388	7)	(389	4)	(423	3)	(436	3)	(444	5)
(445	24)	(446	11)	(447	6)	(513	3)	(589	6)

NAME:12C\_2339.5\_1160EC23\_[882; Pseudouridine (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:234001-10-1

RI:2340

RT:14.991

NUM PEAKS: 133

( 70	4)	( 72	16)	( 73	1000)	( 74	79)	( 75	31)
( 82	3)	( 86	4)	( 89	8)	( 98	1)	( 99	6)
(100	30)	(101	13)	(103	86)	(104	6)	(105	3)
(106	5)	(111	5)	(113	6)	(115	2)	(116	3)
(117	12)	(119	4)	(122	1)	(125	5)	(126	1)
(127	17)	(128	1)	(129	35)	(130	3)	(131	24)
(132	3)	(133	47)	(134	5)	(135	2)	(136	1)
(140	3)	(141	2)	(142	7)	(143	30)	(144	5)
(145	3)	(147	159)	(148	24)	(149	17)	(151	2)
(154	3)	(157	6)	(158	6)	(159	1)	(166	2)
(172	2)	(177	2)	(179	1)	(180	1)	(184	1)
(185	2)	(186	2)	(189	13)	(191	7)	(192	3)
(193	2)	(198	2)	(201	2)	(202	5)	(203	3)
(204	5)	(207	2)	(209	2)	(211	1)	(215	26)



211

(216	7)	(217	498)	(218	97)	(219	44)	(220	4)
(221	2)	(225	2)	(229	1)	(230	18)	(231	3)
(239	4)	(252	1)	(253	5)	(254	2)	(255	4)
(257	3)	(265	2)	(266	1)	(267	10)	(268	2)
(269	25)	(270	6)	(281	4)	(282	2)	(283	7)
(285	1)	(327	2)	(329	1)	(355	13)	(356	9)
(357	64)	(358	22)	(359	10)	(369	3)	(370	3)
(371	9)	(372	5)	(373	2)	(382	2)	(383	9)
(384	5)	(385	2)	(386	4)	(409	2)	(410	1)
(411	10)	(412	5)	(423	5)	(424	32)	(425	18)
(426	8)	(443	1)	(496	6)	(497	5)	(498	2)
(499	3)	(500	2)	(501	2)	(513	1)	(514	3)
(589	5)	(590	2)	(591	2)				

NAME:12C\_2651.1\_1160EC15\_[721; Adenosine (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:265001-10-1

RI:2651

RT:16.639

NUM PEAKS: 46

( 73	1000)	( 74	67)	( 76	6)	( 79	15)	(101	15)
(103	102)	(110	12)	(116	5)	(129	17)	(133	46)
(143	28)	(147	115)	(148	6)	(157	10)	(169	19)
(186	5)	(192	76)	(202	5)	(204	21)	(206	22)
(208	59)	(217	134)	(218	35)	(230	199)	(231	35)
(236	182)	(237	39)	(243	34)	(245	92)	(246	19)
(259	14)	(266	24)	(279	12)	(287	6)	(322	28)
(335	15)	(374	3)	(375	7)	(385	8)	(463	8)
(475	16)	(495	5)	(502	5)	(519	9)	(524	6)
(540	8)								

NAME:12C\_1924.2\_1313EC57\_Mannitol (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:193002-10-1

RI:1924

RT:12.009

NUM PEAKS: 126

( 70	2)	( 72	14)	( 73	1000)	( 74	88)	( 75	45)
( 83	11)	( 87	6)	( 88	5)	( 89	31)	( 90	3)
( 97	9)	( 99	4)	(101	25)	(102	4)	(103	188)
(104	16)	(111	2)	(113	4)	(115	4)	(116	5)
(117	120)	(118	11)	(119	9)	(127	2)	(129	93)
(130	10)	(131	32)	(132	3)	(133	60)	(134	8)
(135	5)	(141	2)	(142	1)	(143	13)	(144	2)
(145	4)	(147	324)	(148	49)	(149	26)	(150	3)
(151	2)	(157	64)	(158	8)	(159	4)	(161	3)
(163	3)	(169	6)	(170	1)	(175	5)	(177	2)
(183	6)	(186	1)	(189	43)	(190	10)	(191	42)
(192	6)	(193	2)	(203	4)	(204	46)	(205	167)
(206	32)	(207	13)	(215	1)	(216	2)	(217	167)
(218	34)	(219	15)	(220	1)	(221	5)	(222	1)
(229	17)	(230	6)	(231	17)	(232	4)	(233	1)
(239	1)	(246	1)	(249	1)	(250	1)	(252	1)
(255	7)	(256	2)	(257	1)	(259	6)	(260	1)
(277	6)	(278	3)	(279	1)	(291	6)	(292	3)
(293	1)	(305	7)	(306	5)	(307	21)	(308	7)
(309	2)	(318	9)	(319	140)	(320	47)	(321	20)
(322	4)	(323	1)	(329	1)	(330	2)	(331	16)
(332	6)	(333	2)	(334	1)	(345	5)	(346	2)
(397	1)	(409	1)	(419	2)	(420	2)	(421	4)

212

(422 1) (423 1) (424 1) (433 1) (477 1)  
 (485 1) (525 1) (526 1) (529 1) (552 1)  
 (579 1)

NAME:12C\_1920.1\_1313EC57\_[529; Methylcitric acid (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:192007-10-1

RI:1920

RT:11.983

NUM PEAKS: 157

( 72 34) ( 73 1000) ( 74 107) ( 75 160) ( 76 8)  
 ( 77 7) ( 80 2) ( 81 13) ( 83 4) ( 89 11)  
 ( 90 3) ( 91 5) ( 92 2) ( 97 16) ( 99 8)  
 (101 15) (104 7) (105 11) (109 8) (116 16)  
 (118 7) (119 7) (122 2) (125 35) (127 6)  
 (129 29) (131 41) (133 77) (134 11) (135 10)  
 (136 3) (141 3) (143 12) (144 5) (145 4)  
 (147 314) (148 50) (149 53) (150 6) (151 3)  
 (152 2) (153 11) (155 22) (159 2) (161 3)  
 (163 3) (169 12) (170 3) (171 16) (173 7)  
 (181 5) (183 3) (185 3) (189 13) (190 6)  
 (192 3) (193 2) (197 30) (198 4) (199 9)  
 (203 6) (204 29) (207 7) (208 2) (209 3)  
 (210 2) (215 4) (216 3) (218 18) (219 6)  
 (221 19) (222 3) (225 5) (226 2) (227 3)  
 (242 3) (243 50) (244 12) (245 11) (246 2)  
 (247 1) (248 1) (249 2) (251 1) (252 2)  
 (259 4) (271 7) (273 2) (278 2) (286 3)  
 (287 106) (288 27) (289 11) (290 3) (291 3)  
 (292 2) (293 2) (299 6) (300 1) (301 2)  
 (305 4) (310 1) (314 1) (315 1) (325 3)  
 (332 3) (333 3) (334 3) (335 1) (336 2)  
 (337 1) (345 1) (347 3) (359 1) (360 4)  
 (361 20) (362 6) (376 2) (377 10) (378 3)  
 (386 2) (387 1) (388 1) (389 5) (403 1)  
 (404 1) (408 1) (409 1) (410 1) (411 1)  
 (414 2) (424 1) (429 1) (430 1) (439 2)  
 (443 1) (449 1) (453 1) (456 1) (461 3)  
 (477 1) (478 4) (479 7) (480 4) (481 3)  
 (482 1) (485 1) (493 2) (496 2) (497 2)  
 (508 1) (510 1) (526 2) (529 1) (547 1)  
 (555 1) (558 1)

NAME:12C\_1544.5\_1313EC75\_Erythronic acid (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:154001-10-1

RI:1545

RT:9.099

NUM PEAKS: 72

( 70 335) ( 71 4) ( 72 13) ( 73 1000) ( 74 78)  
 ( 83 10) ( 89 22) ( 99 5) (101 12) (102 92)  
 (103 103) (104 12) (112 122) (113 11) (117 148)  
 (118 12) (119 13) (129 35) (130 74) (131 35)  
 (132 8) (133 70) (134 8) (135 6) (136 2)  
 (139 2) (143 33) (144 9) (147 485) (148 79)  
 (149 44) (150 5) (152 3) (163 5) (167 2)  
 (177 17) (178 4) (180 6) (181 3) (185 3)  
 (189 22) (190 3) (196 1) (203 7) (204 18)  
 (205 100) (206 18) (214 35) (215 2) (217 84)  
 (218 16) (219 12) (220 121) (229 10) (239 6)

213

(241	7)	(242	2)	(254	26)	(255	5)	(256	2)
(269	3)	(291	19)	(292	138)	(293	41)	(294	17)
(305	2)	(319	8)	(320	2)	(321	2)	(379	2)
(409	3)	(535	1)						

NAME:12C\_1291.0\_1185EK01\_Leucine (2TMS)  
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
 CASNO:129002-01-1  
 RI:1291

NUM PEAKS: 98

( 70	21)	( 71	10)	( 72	27)	( 73	1000)	( 74	112)
( 75	178)	( 76	14)	( 77	55)	( 78	5)	( 79	8)
( 80	2)	( 81	1)	( 82	4)	( 83	3)	( 84	13)
( 85	7)	( 86	46)	( 87	10)	( 88	4)	( 89	4)
( 90	1)	( 91	1)	( 92	2)	( 93	1)	( 94	1)
( 95	1)	( 96	5)	( 97	3)	( 98	6)	( 99	10)
(100	89)	(101	17)	(102	168)	(103	44)	(104	9)
(105	5)	(110	1)	(111	1)	(112	3)	(113	2)
(114	4)	(115	25)	(116	32)	(117	25)	(118	5)
(119	5)	(126	2)	(127	1)	(128	23)	(129	9)
(130	41)	(131	19)	(132	20)	(133	41)	(134	7)
(135	3)	(140	1)	(142	14)	(143	4)	(144	5)
(145	1)	(146	4)	(147	117)	(148	19)	(149	10)
(150	1)	(156	3)	(157	2)	(158	720)	(159	105)
(160	32)	(161	3)	(163	1)	(170	8)	(171	2)
(172	1)	(174	3)	(175	2)	(176	2)	(177	2)
(186	1)	(188	1)	(191	1)	(202	1)	(203	3)
(204	2)	(205	4)	(206	1)	(207	1)	(218	21)
(219	5)	(220	2)	(231	1)	(232	25)	(233	6)
(234	2)	(260	7)	(261	2)				

NAME:12C\_1273.1\_1313EC43\_[938; Sulfuric acid (2TMS)]  
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer  
 CASNO:127005-10-1  
 RI:1273

RT:6.066

NUM PEAKS: 344

( 72	37)	( 73	278)	( 74	26)	( 76	10)	( 83	5)
( 84	13)	( 88	7)	( 89	23)	( 90	7)	( 94	4)
( 95	11)	( 98	7)	(107	12)	(108	9)	(109	7)
(111	6)	(112	6)	(113	5)	(114	15)	(115	17)
(116	16)	(118	12)	(119	13)	(120	9)	(122	9)
(123	18)	(125	12)	(128	6)	(130	4)	(132	30)
(133	33)	(134	18)	(137	5)	(138	10)	(139	28)
(140	8)	(141	10)	(143	7)	(144	4)	(145	9)
(147	1000)	(148	179)	(149	106)	(150	17)	(151	7)
(152	7)	(153	6)	(154	8)	(155	4)	(156	6)
(158	7)	(159	9)	(160	6)	(162	10)	(164	4)
(165	5)	(168	9)	(169	7)	(170	6)	(171	6)
(172	5)	(173	5)	(177	6)	(181	7)	(182	8)
(184	7)	(185	5)	(186	9)	(187	7)	(188	7)
(189	6)	(190	6)	(191	7)	(193	3)	(194	4)
(197	8)	(198	7)	(201	5)	(202	6)	(205	8)
(206	3)	(208	6)	(209	6)	(210	6)	(211	8)
(216	6)	(217	8)	(218	6)	(222	5)	(223	6)
(224	4)	(226	7)	(227	187)	(228	32)	(229	28)
(230	11)	(233	4)	(234	2)	(235	5)	(236	8)
(237	7)	(238	6)	(239	6)	(240	7)	(241	6)
(242	7)	(243	8)	(244	6)	(245	8)	(247	8)
(249	6)	(250	6)	(252	8)	(253	7)	(254	9)

214

(255	8)	(256	8)	(257	4)	(258	8)	(262	7)
(263	7)	(264	4)	(265	8)	(267	9)	(270	8)
(271	9)	(272	9)	(275	9)	(277	11)	(279	12)
(280	12)	(281	9)	(282	10)	(283	8)	(284	7)
(288	9)	(289	7)	(292	7)	(293	8)	(296	5)
(297	8)	(300	9)	(301	6)	(302	10)	(303	3)
(306	4)	(308	3)	(309	4)	(310	5)	(311	4)
(313	5)	(314	4)	(316	8)	(317	6)	(319	5)
(320	4)	(322	7)	(325	6)	(326	9)	(327	6)
(328	10)	(329	8)	(330	9)	(331	7)	(332	7)
(333	8)	(334	5)	(335	6)	(336	6)	(338	5)
(341	6)	(342	7)	(345	6)	(346	7)	(347	8)
(348	7)	(349	7)	(350	6)	(351	9)	(352	6)
(353	9)	(354	12)	(355	6)	(356	9)	(358	11)
(360	4)	(361	7)	(362	8)	(363	13)	(369	12)
(373	8)	(374	8)	(375	15)	(376	8)	(381	9)
(382	7)	(383	7)	(384	11)	(385	10)	(386	12)
(388	10)	(389	12)	(393	6)	(394	6)	(395	9)
(396	16)	(398	7)	(400	11)	(401	10)	(402	9)
(403	8)	(406	8)	(407	9)	(408	8)	(409	7)
(410	7)	(411	4)	(415	7)	(416	8)	(417	8)
(418	7)	(419	5)	(420	7)	(421	6)	(422	7)
(423	4)	(424	6)	(425	10)	(426	4)	(428	5)
(429	7)	(430	10)	(431	8)	(432	4)	(433	4)
(435	5)	(436	7)	(439	6)	(440	6)	(441	10)
(442	7)	(443	5)	(444	5)	(445	7)	(446	6)
(449	8)	(452	9)	(453	10)	(454	8)	(457	4)
(458	7)	(459	10)	(460	11)	(462	8)	(463	10)
(465	10)	(466	12)	(467	7)	(468	9)	(469	8)
(470	11)	(471	8)	(472	6)	(474	8)	(475	6)
(476	7)	(477	10)	(478	9)	(479	6)	(481	9)
(482	11)	(483	5)	(484	6)	(485	8)	(486	14)
(487	9)	(488	7)	(489	5)	(492	8)	(494	10)
(495	7)	(496	11)	(498	8)	(499	11)	(500	11)
(502	11)	(503	10)	(505	6)	(506	12)	(509	4)
(510	6)	(511	6)	(512	8)	(513	8)	(514	5)
(516	7)	(517	12)	(518	8)	(519	5)	(521	7)
(522	9)	(523	5)	(524	7)	(525	5)	(526	9)
(528	9)	(529	12)	(530	6)	(531	7)	(532	7)
(533	7)	(534	7)	(535	9)	(536	4)	(537	11)
(538	8)	(539	4)	(541	7)	(545	6)	(546	4)
(548	9)	(549	8)	(551	5)	(552	7)	(553	2)
(555	5)	(556	3)	(557	4)	(558	7)	(559	4)
(561	6)	(563	3)	(564	4)	(565	4)	(567	3)
(570	5)	(572	6)	(573	4)	(578	4)	(579	4)
(580	3)	(583	3)	(589	5)	(595	2)		

NAME:12C\_1269.8\_1135EC44\_Urea (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:127002-01-1

RI:1270

RT:402.296

RSN:2975.0

NUM PEAKS: 51

( 70	62)	( 71	56)	( 72	79)	( 73	377)	( 74	147)
( 75	115)	( 76	11)	( 77	6)	( 78	21)	( 79	64)
( 80	5)	( 84	10)	( 85	24)	( 86	21)	( 87	78)
( 88	10)	( 90	6)	( 99	136)	(100	100)	(101	33)
(102	20)	(103	12)	(105	8)	(111	5)	(113	15)
(114	15)	(115	31)	(116	12)	(117	6)	(130	68)

## 215

(131 67) (132 56) (133 31) (134 6) (146 66)  
 (147 1000) (148 161) (149 78) (150 7) (155 4)  
 (157 15) (171 158) (172 29) (173 65) (174 11)  
 (175 4) (186 9) (189 434) (190 79) (191 35)  
 (204 21)

NAME:12C\_1723.7\_1160EC15\_2-Aminoadipic acid (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:172006-10-1

RI:1724

RT:10.996

NUM PEAKS: 183

( 70 20) ( 71 15) ( 72 35) ( 73 1000) ( 74 100)  
 ( 75 283) ( 76 21) ( 77 23) ( 78 5) ( 79 9)  
 ( 80 12) ( 81 8) ( 82 6) ( 83 11) ( 85 28)  
 ( 86 15) ( 87 9) ( 88 5) ( 89 6) ( 91 2)  
 ( 92 1) ( 93 15) ( 94 2) ( 95 9) ( 96 8)  
 ( 97 20) ( 98 47) ( 99 17) (100 135) (101 24)  
 (102 12) (104 5) (107 2) (108 10) (109 3)  
 (110 3) (111 9) (112 9) (113 4) (114 13)  
 (115 86) (116 30) (117 29) (118 5) (119 7)  
 (121 1) (122 1) (123 4) (124 2) (125 2)  
 (126 5) (127 4) (128 219) (129 199) (130 36)  
 (131 53) (132 23) (133 58) (134 9) (135 6)  
 (136 1) (137 3) (138 3) (141 2) (142 8)  
 (143 7) (144 2) (145 6) (146 3) (147 178)  
 (148 31) (149 39) (150 6) (151 14) (152 4)  
 (153 4) (154 33) (159 3) (161 2) (162 1)  
 (163 12) (164 3) (165 1) (168 3) (169 1)  
 (170 37) (171 6) (172 13) (174 10) (175 2)  
 (182 13) (183 3) (187 1) (188 11) (193 2)  
 (198 1) (200 2) (202 8) (203 18) (208 1)  
 (213 2) (216 4) (217 304) (218 87) (219 34)  
 (220 5) (221 6) (228 8) (231 1) (232 2)  
 (233 2) (234 1) (235 1) (242 2) (243 11)  
 (244 71) (245 18) (246 8) (250 1) (251 1)  
 (252 1) (254 2) (256 1) (259 3) (260 357)  
 (261 83) (262 33) (263 5) (266 1) (272 28)  
 (273 6) (274 3) (278 1) (286 1) (287 1)  
 (288 6) (289 2) (290 1) (291 7) (292 2)  
 (293 2) (294 1) (301 2) (302 2) (313 1)  
 (317 1) (318 1) (326 1) (334 3) (335 2)  
 (337 1) (342 1) (348 1) (361 1) (362 15)  
 (363 6) (364 3) (376 1) (377 9) (378 4)  
 (379 1) (391 1) (393 1) (417 1) (418 2)  
 (428 1) (438 1) (450 1) (465 1) (472 1)  
 (478 1) (486 1) (497 1) (503 1) (513 1)  
 (523 1) (529 1) (532 1) (537 1) (540 1)  
 (541 1) (547 1) (562 1)

NAME:12C\_1739.1\_1274EC11\_Aspartic acid (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:174003-10-1

RI:1739

RT:11.121

NUM PEAKS: 117

( 70 40) ( 71 24) ( 72 30) ( 73 1000) ( 74 102)  
 ( 79 20) ( 80 14) ( 88 6) ( 89 30) ( 92 5)  
 ( 94 9) ( 96 9) ( 98 9) ( 99 46) (100 58)  
 (105 24) (106 9) (107 5) (108 4) (113 7)

## 216

(114	10)	(121	4)	(124	5)	(127	21)	(130	26)
(131	23)	(133	89)	(134	11)	(135	5)	(141	13)
(142	8)	(143	22)	(144	6)	(145	4)	(146	13)
(149	25)	(150	10)	(157	22)	(158	19)	(159	36)
(160	11)	(161	8)	(162	3)	(163	83)	(164	17)
(169	12)	(171	16)	(172	75)	(173	25)	(177	7)
(183	10)	(185	18)	(188	6)	(191	26)	(197	4)
(199	10)	(202	33)	(205	243)	(206	45)	(207	23)
(213	6)	(215	34)	(216	13)	(221	26)	(222	9)
(223	7)	(242	4)	(244	8)	(246	6)	(247	6)
(257	5)	(259	6)	(262	5)	(264	4)	(273	26)
(275	9)	(276	5)	(279	21)	(280	9)	(287	12)
(288	21)	(289	22)	(290	24)	(291	8)	(299	8)
(302	5)	(304	31)	(306	7)	(316	5)	(317	7)
(330	7)	(331	13)	(332	6)	(347	8)	(363	14)
(364	7)	(365	5)	(378	8)	(379	5)	(380	6)
(382	3)	(406	14)	(407	10)	(421	3)	(422	5)
(424	7)	(430	5)	(432	5)	(454	6)	(498	7)
(506	4)	(511	5)	(519	4)	(527	4)	(529	4)
(553	4)	(565	4)						

NAME:12C\_2225.6\_1178EC20\_Tryptophan (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:223001-10-1

RI:2226

RT:14.362

NUM PEAKS: 95

( 72	12)	( 73	1000)	( 76	6)	( 77	12)	( 91	3)
( 92	3)	( 94	3)	( 96	25)	(100	13)	(103	3)
(105	8)	(106	3)	(110	8)	(116	15)	(122	3)
(124	3)	(128	7)	(129	32)	(130	19)	(131	41)
(132	42)	(133	21)	(134	8)	(138	3)	(142	3)
(145	48)	(146	17)	(147	29)	(148	5)	(152	7)
(155	3)	(156	9)	(159	9)	(160	8)	(161	6)
(170	3)	(173	5)	(175	3)	(180	8)	(184	6)
(187	12)	(188	8)	(189	7)	(190	8)	(200	11)
(201	5)	(202	705)	(203	155)	(204	45)	(215	8)
(218	17)	(219	30)	(220	10)	(221	5)	(222	5)
(229	3)	(230	8)	(231	7)	(232	3)	(233	4)
(235	7)	(236	3)	(246	3)	(248	3)	(257	3)
(261	4)	(264	6)	(265	6)	(291	38)	(292	15)
(293	6)	(303	4)	(327	4)	(337	4)	(338	4)
(351	4)	(367	3)	(379	3)	(394	3)	(406	4)
(407	8)	(408	9)	(409	3)	(421	3)	(422	10)
(423	8)	(424	4)	(425	3)	(427	3)	(437	4)
(446	3)	(462	5)	(496	3)	(542	3)	(564	3)

NAME:12C\_2770.4\_1160EC15\_[626; 5'-Methylthioadenosine (3TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:277004-10-1

RI:2770

RT:17.269

NUM PEAKS: 24

( 73	1000)	( 74	105)	( 87	43)	(101	75)	(108	46)
(115	35)	(116	53)	(119	32)	(127	34)	(135	63)
(136	276)	(137	30)	(148	36)	(164	692)	(165	43)
(169	261)	(175	769)	(176	98)	(177	35)	(188	441)
(190	35)	(208	45)	(234	13)	(426	28)		

NAME:12C\_1324.1\_1313EC07\_Nicotinic acid (1TMS)

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COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:133004-10-1

RI:1324

RT:6.689

NUM PEAKS: 17

( 78	769)	( 79	88)	( 83	111)	(106	622)	(107	47)
(110	11)	(111	38)	(112	48)	(136	836)	(137	90)
(138	26)	(141	49)	(180	1000)	(181	149)	(182	36)
(186	61)	(195	41)						

NAME:12C\_2427.5\_1313EC07\_[931; myo-Inositol-1-phosphate (7TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:243001-10-1

RI:2428

RT:14.977

NUM PEAKS: 283

( 70	3)	( 71	3)	( 72	16)	( 73	1000)	( 74	89)
( 75	76)	( 76	4)	( 77	10)	( 78	1)	( 79	3)
( 80	1)	( 81	14)	( 82	2)	( 83	4)	( 84	1)
( 85	5)	( 86	2)	( 87	6)	( 88	2)	( 89	5)
( 90	1)	( 91	3)	( 92	1)	( 93	2)	( 94	1)
( 95	2)	( 96	2)	( 97	2)	( 98	2)	( 99	5)
(100	1)	(101	8)	(102	4)	(103	25)	(105	6)
(106	2)	(107	3)	(108	1)	(109	5)	(110	1)
(111	6)	(112	1)	(113	5)	(114	1)	(115	7)
(116	5)	(117	7)	(118	1)	(119	6)	(120	1)
(121	3)	(123	1)	(125	2)	(126	1)	(127	6)
(128	1)	(129	36)	(130	4)	(131	21)	(132	4)
(133	64)	(134	9)	(135	13)	(136	2)	(137	6)
(138	1)	(139	2)	(140	1)	(141	3)	(142	3)
(143	18)	(144	2)	(145	3)	(146	1)	(147	252)
(148	41)	(149	26)	(150	3)	(151	6)	(152	1)
(153	5)	(154	2)	(155	5)	(156	4)	(157	5)
(158	1)	(159	2)	(160	1)	(161	3)	(162	1)
(163	3)	(164	1)	(165	2)	(166	1)	(167	2)
(168	1)	(169	5)	(170	1)	(171	1)	(173	1)
(175	3)	(176	1)	(177	3)	(178	1)	(179	2)
(180	1)	(181	8)	(182	2)	(183	4)	(184	1)
(185	1)	(187	1)	(189	8)	(190	7)	(191	47)
(192	9)	(193	12)	(194	2)	(195	4)	(196	1)
(197	2)	(199	1)	(201	2)	(202	1)	(203	2)
(204	15)	(205	7)	(206	2)	(207	15)	(208	4)
(209	3)	(210	2)	(211	35)	(212	6)	(213	4)
(214	1)	(215	4)	(216	2)	(217	46)	(218	10)
(219	4)	(221	8)	(222	2)	(223	1)	(224	1)
(225	9)	(226	2)	(227	11)	(228	3)	(229	2)
(230	11)	(231	4)	(232	1)	(233	1)	(235	1)
(237	1)	(239	2)	(240	1)	(241	2)	(242	1)
(243	11)	(244	3)	(245	3)	(246	9)	(247	2)
(248	1)	(249	1)	(251	1)	(252	1)	(253	1)
(254	1)	(255	8)	(256	2)	(257	3)	(258	1)
(259	1)	(265	3)	(266	1)	(267	1)	(268	1)
(269	3)	(270	2)	(271	3)	(272	1)	(273	1)
(278	1)	(283	4)	(284	2)	(285	7)	(286	2)
(287	1)	(291	5)	(292	2)	(293	1)	(297	1)
(298	12)	(299	108)	(300	32)	(301	17)	(302	3)
(303	1)	(304	2)	(305	8)	(306	4)	(307	2)
(308	1)	(312	1)	(313	4)	(314	11)	(315	89)
(316	26)	(317	25)	(318	104)	(319	35)	(320	15)
(321	3)	(322	1)	(327	1)	(328	1)	(329	1)

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(330	1)	(331	2)	(332	1)	(333	1)	(340	1)
(341	2)	(342	3)	(343	8)	(344	4)	(345	5)
(346	2)	(347	1)	(357	1)	(358	1)	(359	1)
(360	1)	(367	1)	(368	1)	(369	1)	(370	1)
(371	1)	(372	2)	(373	6)	(374	3)	(375	1)
(385	2)	(386	11)	(387	39)	(388	19)	(389	19)
(390	6)	(391	3)	(392	1)	(417	1)	(418	1)
(419	2)	(420	1)	(421	1)	(428	1)	(429	3)
(430	1)	(431	2)	(432	5)	(433	4)	(434	2)
(435	1)	(441	1)	(442	1)	(443	1)	(444	1)
(455	1)	(456	1)	(457	1)	(458	1)	(459	1)
(460	1)	(461	1)	(462	1)	(469	1)	(470	2)
(471	1)	(472	1)	(507	1)				

NAME:12C\_2000.0\_1313EC07\_Panthotenic acid (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:200006-10-1

RI:2000

RT:12.490

NUM PEAKS: 107

( 78	209)	( 79	192)	( 80	14)	(108	92)	(109	16)
(123	74)	(124	132)	(127	69)	(128	70)	(129	254)
(143	25)	(157	1000)	(166	33)	(170	38)	(182	1)
(184	30)	(185	15)	(197	4)	(198	16)	(201	777)
(202	71)	(247	119)	(274	8)	(284	7)	(285	26)
(286	9)	(290	82)	(291	871)	(292	113)	(330	17)
(346	72)	(347	28)	(359	43)	(360	3)	(361	18)
(374	21)	(375	21)	(386	18)	(390	14)	(391	15)
(406	68)	(420	168)	(421	85)	(433	7)	(434	44)
(445	66)	(446	27)	(448	20)	(449	1)	(450	5)
(463	50)	(465	16)	(467	4)	(468	5)	(475	3)
(480	18)	(481	13)	(482	53)	(487	55)	(493	34)
(494	12)	(496	29)	(497	17)	(502	9)	(505	28)
(506	19)	(510	5)	(511	55)	(514	35)	(515	15)
(516	7)	(519	67)	(522	73)	(523	12)	(524	49)
(525	1)	(526	3)	(534	60)	(539	64)	(540	13)
(543	76)	(545	5)	(547	57)	(548	15)	(549	20)
(551	20)	(552	68)	(553	1)	(557	14)	(562	4)
(563	6)	(569	8)	(570	37)	(575	6)	(577	26)
(579	13)	(580	16)	(582	12)	(583	25)	(585	13)
(586	14)	(588	28)	(591	12)	(593	12)	(595	10)
(596	14)	(597	2)						

NAME:12C\_1292.9\_1313EC11\_Leucine (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:129002-10-1

RI:1293

RT:6.287

NUM PEAKS: 4

( 79 83) (158 1000) (159 20) (232 2)

NAME:12C\_1490.1\_2119DC04\_[545; 2,3-Dimethylsuccinic acid (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:149003-10-1

RI:1490

RT:20.245

NUM PEAKS: 166

( 41	217)	( 42	21)	( 43	227)	( 44	61)	( 45	122)
( 47	52)	( 50	20)	( 52	23)	( 53	34)	( 54	11)
( 57	15)	( 58	41)	( 59	316)	( 60	26)	( 61	65)



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( 62	6)	( 63	11)	( 65	17)	( 66	6)	( 67	79)
( 68	21)	( 69	185)	( 70	11)	( 71	52)	( 72	11)
( 73	408)	( 74	32)	( 75	1000)	( 76	82)	( 77	49)
( 79	35)	( 81	30)	( 82	19)	( 83	116)	( 84	6)
( 85	123)	( 86	13)	( 89	734)	( 90	61)	( 91	64)
( 92	7)	( 93	8)	( 95	128)	( 96	18)	( 97	46)
( 98	10)	( 99	55)	(103	19)	(105	44)	(107	8)
(108	2)	(110	4)	(111	9)	(113	267)	(114	22)
(119	9)	(120	4)	(123	15)	(125	17)	(127	72)
(131	84)	(132	11)	(137	7)	(139	2)	(141	20)
(143	479)	(144	55)	(145	114)	(146	42)	(147	826)
(148	134)	(149	30)	(154	5)	(155	79)	(156	11)
(157	278)	(158	38)	(159	237)	(160	27)	(161	85)
(162	24)	(163	355)	(164	53)	(165	34)	(166	7)
(169	8)	(170	18)	(173	41)	(174	13)	(179	3)
(180	6)	(185	31)	(186	8)	(187	44)	(191	310)
(192	43)	(193	30)	(196	4)	(197	3)	(201	59)
(207	435)	(208	64)	(209	47)	(210	7)	(212	2)
(213	5)	(215	14)	(216	7)	(217	12)	(226	3)
(229	72)	(231	184)	(232	33)	(239	2)	(244	2)
(247	174)	(248	36)	(249	20)	(250	5)	(254	5)
(258	3)	(259	28)	(261	24)	(262	3)	(270	3)
(271	3)	(275	362)	(276	92)	(277	35)	(278	5)
(291	87)	(292	21)	(293	7)	(299	4)	(301	2)
(313	3)	(319	46)	(320	10)	(321	2)	(322	2)
(333	3)	(346	2)	(354	2)	(356	2)	(371	2)
(380	3)	(388	2)	(397	2)	(407	3)	(434	2)
(439	3)	(453	2)	(466	3)	(476	2)	(479	3)
(515	2)	(521	2)	(527	2)	(533	2)	(552	2)
(562	3)	(567	2)	(579	2)	(594	2)	(596	5)
(598	7)								

NAME:12C\_2816.0\_2119DC04\_[542; Maltose methoxyamine {BP} (8TMS); alpha-D-Glc-(1,4)-alpha-D-Glc]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:282003-10-1

RI:2816

RT:41.182

NUM PEAKS: 75

( 44	171)	( 48	62)	( 64	42)	( 73	1000)	( 82	73)
( 88	62)	(103	130)	(104	92)	(108	67)	(111	127)
(129	273)	(130	78)	(133	147)	(143	44)	(147	245)
(152	34)	(167	53)	(169	195)	(172	33)	(175	40)
(179	127)	(181	52)	(191	520)	(192	167)	(197	50)
(202	43)	(207	109)	(214	26)	(215	29)	(217	105)
(218	44)	(220	30)	(229	57)	(236	29)	(241	39)
(242	28)	(243	110)	(244	76)	(246	29)	(251	35)
(252	59)	(267	42)	(270	47)	(275	32)	(281	53)
(319	64)	(321	44)	(323	32)	(333	45)	(353	24)
(357	55)	(361	166)	(362	69)	(363	56)	(386	29)
(393	25)	(400	22)	(407	40)	(431	37)	(439	27)
(443	24)	(457	24)	(464	36)	(469	41)	(488	29)
(506	37)	(507	25)	(509	37)	(521	27)	(523	25)
(530	33)	(550	24)	(581	26)	(587	26)	(597	24)

NAME:12C\_1685.1\_1313EC57\_Ribose methoxyamine (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1685 |RI:1685 |RI:1685

CASNO:168002-10-1

RI:1685

RT:10.186

SOURCE: C:\NISTMS\AMDIS32\LIB\MS\_RI.msp

NUM PEAKS: 431

( 70	75)	( 71	28)	( 73	1000)	( 74	24)	( 78	10)
( 82	16)	( 83	39)	( 84	24)	( 85	16)	( 86	7)
( 87	13)	( 88	10)	( 89	66)	( 90	11)	( 91	28)
( 92	6)	( 95	5)	( 96	4)	( 97	4)	( 98	8)
( 99	17)	(101	33)	(102	5)	(103	282)	(104	31)
(105	37)	(106	6)	(107	4)	(108	2)	(109	21)
(111	5)	(112	10)	(113	17)	(117	59)	(119	18)
(120	5)	(121	5)	(122	4)	(123	4)	(126	9)
(127	8)	(128	18)	(129	43)	(133	69)	(135	8)
(136	2)	(137	6)	(138	5)	(139	5)	(140	15)
(143	6)	(144	40)	(145	19)	(147	244)	(148	42)
(149	17)	(151	6)	(152	4)	(153	4)	(155	55)
(156	12)	(157	8)	(158	10)	(160	127)	(161	23)
(162	11)	(163	11)	(164	6)	(165	4)	(166	3)
(167	7)	(168	6)	(170	7)	(171	4)	(172	7)
(173	27)	(174	19)	(175	12)	(176	5)	(177	6)
(178	5)	(179	3)	(181	5)	(182	7)	(183	5)
(184	7)	(186	6)	(187	7)	(189	44)	(190	17)
(191	17)	(192	6)	(194	6)	(195	7)	(196	5)
(197	6)	(198	6)	(199	12)	(200	18)	(201	9)
(203	8)	(204	16)	(205	34)	(206	12)	(207	5)
(208	4)	(209	5)	(210	3)	(212	4)	(213	11)
(216	8)	(217	133)	(218	30)	(219	16)	(221	6)
(222	5)	(223	5)	(224	3)	(225	3)	(228	4)
(229	5)	(230	8)	(233	19)	(234	8)	(235	5)
(236	3)	(237	4)	(239	2)	(240	6)	(241	2)
(242	6)	(245	12)	(246	7)	(247	5)	(248	6)
(249	3)	(250	6)	(251	5)	(252	4)	(254	6)
(255	4)	(256	6)	(257	7)	(260	3)	(261	4)
(262	9)	(263	15)	(264	8)	(265	6)	(266	5)
(267	4)	(268	6)	(269	5)	(270	5)	(271	6)
(272	5)	(273	4)	(274	5)	(276	6)	(277	14)
(278	6)	(279	6)	(280	3)	(281	5)	(282	5)
(283	3)	(284	4)	(285	3)	(286	6)	(287	10)
(289	5)	(290	31)	(291	15)	(292	8)	(293	6)
(294	5)	(295	5)	(296	5)	(297	5)	(298	4)
(299	7)	(300	5)	(302	7)	(303	3)	(304	2)
(306	3)	(307	42)	(308	15)	(309	9)	(310	6)
(311	4)	(313	3)	(314	3)	(315	2)	(317	3)
(318	4)	(319	6)	(322	3)	(323	3)	(324	4)
(325	4)	(326	4)	(327	5)	(328	3)	(329	2)
(330	3)	(331	4)	(332	6)	(335	5)	(336	4)
(337	5)	(338	5)	(339	4)	(342	3)	(343	2)
(344	2)	(345	2)	(346	3)	(347	4)	(349	4)
(350	2)	(351	4)	(352	7)	(353	5)	(354	3)
(355	2)	(357	3)	(358	5)	(359	4)	(360	5)
(361	3)	(362	5)	(363	2)	(364	6)	(365	7)
(366	6)	(367	6)	(368	4)	(370	3)	(371	3)
(372	5)	(373	5)	(374	4)	(375	2)	(377	4)
(379	3)	(380	4)	(381	6)	(382	4)	(383	4)
(384	3)	(385	3)	(386	3)	(387	5)	(388	4)
(389	3)	(390	5)	(391	4)	(392	3)	(393	4)
(394	3)	(395	3)	(396	4)	(397	4)	(399	4)
(401	3)	(402	5)	(403	4)	(404	5)	(405	3)
(406	4)	(407	5)	(408	2)	(411	7)	(412	5)
(413	5)	(414	5)	(415	4)	(416	4)	(419	4)
(420	6)	(421	4)	(422	2)	(423	2)	(424	4)
(425	4)	(426	6)	(427	3)	(428	5)	(429	6)

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(430	4)	(431	2)	(432	2)	(434	5)	(435	4)
(436	6)	(437	3)	(439	3)	(440	4)	(442	2)
(443	5)	(444	5)	(445	5)	(446	4)	(447	3)
(448	5)	(449	6)	(450	3)	(451	3)	(452	5)
(453	4)	(454	2)	(455	4)	(456	4)	(457	6)
(458	5)	(459	3)	(460	3)	(461	2)	(462	6)
(463	3)	(465	3)	(466	3)	(467	5)	(468	5)
(469	5)	(470	4)	(471	2)	(474	3)	(475	2)
(477	2)	(478	4)	(479	3)	(480	3)	(481	4)
(482	4)	(483	2)	(484	4)	(485	3)	(486	3)
(487	3)	(489	3)	(490	4)	(491	5)	(492	2)
(493	4)	(494	4)	(496	3)	(497	5)	(498	4)
(499	3)	(500	3)	(501	5)	(502	3)	(503	4)
(504	4)	(505	5)	(506	4)	(507	2)	(509	5)
(510	3)	(511	4)	(512	7)	(513	4)	(514	2)
(515	6)	(516	5)	(517	4)	(518	4)	(519	5)
(520	3)	(521	3)	(523	4)	(524	5)	(525	4)
(526	5)	(527	4)	(528	2)	(529	3)	(530	6)
(531	5)	(532	6)	(533	3)	(534	5)	(536	3)
(537	3)	(538	2)	(539	4)	(540	4)	(541	4)
(542	3)	(543	6)	(544	5)	(545	5)	(546	3)
(547	4)	(548	3)	(549	3)	(550	5)	(551	4)
(552	2)	(553	2)	(555	3)	(556	1)	(557	2)
(558	3)	(559	3)	(560	2)	(561	3)	(562	3)
(563	2)	(564	3)	(565	2)	(566	2)	(567	3)
(569	3)	(570	2)	(571	2)	(572	5)	(574	2)
(575	3)	(577	1)	(578	1)	(579	1)	(580	1)
(582	1)	(583	1)	(588	1)	(590	2)	(592	1)
(593	1)								

NAME:13C\_1685.1\_1313EC16\_Ribose methoxyamine (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1685 |RI:1685 |RI:1685

CASNO:168002-11-1

RI:1685

RT:10.202

SOURCE:C:\NISTMS\AMDIS32\LIB\MS\_RI.msp

NUM PEAKS: 272

( 70	9)	( 71	18)	( 72	34)	( 73	1000)	( 74	136)
( 75	207)	( 76	18)	( 77	15)	( 78	3)	( 79	3)
( 81	1)	( 82	2)	( 83	2)	( 85	21)	( 86	10)
( 87	16)	( 88	12)	( 89	29)	( 90	11)	( 91	26)
( 92	5)	( 95	1)	( 96	1)	( 98	1)	( 99	6)
(100	14)	(101	47)	(102	38)	(103	31)	(104	202)
(105	32)	(106	8)	(108	1)	(109	1)	(113	2)
(114	2)	(115	9)	(116	20)	(117	32)	(118	141)
(119	50)	(120	10)	(121	3)	(122	2)	(127	1)
(128	5)	(129	2)	(130	10)	(131	37)	(132	55)
(133	81)	(134	76)	(135	13)	(136	3)	(138	3)
(139	1)	(141	2)	(142	2)	(143	4)	(144	58)
(145	13)	(146	17)	(147	186)	(148	32)	(149	21)
(150	4)	(151	2)	(153	2)	(156	1)	(157	2)
(158	6)	(159	2)	(160	5)	(161	8)	(162	41)
(163	12)	(164	3)	(165	1)	(167	1)	(168	1)
(169	1)	(172	3)	(173	10)	(174	6)	(175	6)
(176	8)	(177	7)	(178	1)	(179	2)	(181	2)
(187	1)	(188	3)	(189	37)	(190	15)	(191	37)
(192	13)	(193	2)	(194	2)	(196	1)	(197	1)
(201	3)	(202	2)	(203	7)	(204	14)	(205	6)
(206	16)	(207	12)	(208	3)	(209	1)	(211	3)
(212	1)	(216	3)	(217	5)	(218	9)	(219	10)

(220	114)	(221	21)	(222	10)	(224	1)	(225	3)
(226	1)	(230	1)	(232	6)	(233	5)	(234	52)
(235	20)	(236	7)	(237	3)	(238	2)	(239	1)
(245	2)	(247	5)	(248	5)	(252	1)	(255	1)
(257	3)	(259	1)	(261	2)	(262	10)	(263	3)
(264	2)	(265	3)	(266	2)	(267	3)	(268	3)
(269	1)	(270	1)	(271	3)	(272	1)	(274	1)
(276	1)	(278	5)	(279	9)	(280	5)	(281	1)
(283	2)	(285	1)	(286	2)	(287	1)	(293	3)
(294	4)	(295	1)	(297	1)	(298	2)	(299	1)
(302	2)	(303	1)	(304	1)	(307	2)	(308	2)
(309	3)	(310	31)	(311	8)	(312	3)	(313	1)
(314	1)	(315	2)	(316	1)	(317	1)	(320	1)
(324	2)	(325	1)	(326	1)	(327	1)	(333	1)
(334	1)	(337	2)	(338	1)	(341	1)	(342	1)
(346	1)	(348	1)	(351	1)	(352	2)	(353	1)
(357	1)	(360	1)	(361	1)	(362	1)	(363	1)
(368	2)	(369	3)	(370	2)	(372	1)	(373	1)
(377	1)	(380	1)	(385	1)	(386	2)	(387	1)
(390	1)	(393	1)	(394	2)	(395	1)	(401	1)
(407	1)	(416	1)	(418	2)	(419	1)	(421	1)
(425	1)	(426	1)	(427	2)	(428	2)	(435	2)
(436	1)	(439	2)	(443	1)	(446	1)	(447	1)
(450	2)	(451	4)	(452	1)	(453	2)	(454	2)
(455	1)	(462	2)	(463	1)	(466	1)	(467	2)
(471	1)	(479	2)	(483	1)	(487	1)	(492	1)
(494	2)	(508	1)	(509	1)	(510	2)	(511	1)
(513	2)	(516	1)	(523	2)	(525	1)	(528	1)
(529	1)	(530	1)	(531	2)	(537	1)	(538	2)
(542	1)	(550	3)	(554	1)	(558	1)	(559	1)
(560	1)	(563	2)	(566	1)	(574	2)	(582	1)
(588	1)	(590	1)						

223

Table 4

1102.5_1185EK02	999	446	223	312	294	652	348	195	355	191
283	377	360	448	349	367	306	270	366	402	411
341	242	387	462	253	365	386	326	417	388	386
417	410	329	358	344	205	361	511	353	347	267
271	348	365	275	232	302	324	298	330	333	343
315	278	307	290	323	549	284	223	291	249	363
258	319	352	364	211	264	299	377	289	245	312
294	308	341	250	340	312	210	287	318	277	276
287	300	288	312	294	227	309	315	318	272	284
280	296	285	179	291	197	291	291	355	298	294
227	257	258	270	321	256	295	302	219	303	260
237	237	205	276	260	256	220	267	363	325	254
205	317	264	233	330	324	194	328	306	337	170
231	371	246	256	252	253	264	287	276	318	276
252	257	260	295	279	265	289	245	276	254	278
247	187	236	241	311	292	215	248	167	255	252
228	232	243	241	192	202	261	253	232	180	288
371	353	132	227	645	348	390	136	203	420	168
325	339	354	248	267	317	312	384	372	205	495
582	237	448	487	340	330	378	346	311	226	342
267	350	223	238	344	273	272	258	338	292	203
239	0	257	195	332	282	322	306	322	354	51
257	129	552	334	277	322	159	307	332	315	359
164	263	204	341	253	336	287	87	234	326	265
189	326	329	257	221	300	284	284	191	119	324
179	298	292	248	337	208	272	189	287	179	266
0	227	145	270	333	332	281	190	287	317	319
259	287	343	296	258	288	259	261	324	313	256
244	27	283	294	260	376	209	354	337	287	301
230	250	308	348	300	278	190	239	195	268	358
248	222	221	296	301	287	392	252	124	305	223
257	248	1	330	258	131	292	144	295	272	239
212	235	241	242	195	273	246	235	230	206	

224

1140.2_1185EK07	446	999	156	361	341	395	449	192	353	235
304	390	356	547	339	348	340	243	315	403	351
370	241	347	322	256	353	417	376	376	370	347
377	364	301	287	301	182	297	386	304	393	241
256	346	387	261	359	315	293	308	287	313	356
376	271	277	266	310	328	263	252	249	245	273
242	291	280	271	230	283	320	281	293	276	310
248	323	376	268	329	331	294	273	303	297	272
299	291	279	246	325	237	322	353	328	281	278
296	313	328	232	332	230	324	323	336	301	299
232	232	234	236	328	272	328	299	285	298	271
257	283	211	249	251	258	263	295	277	363	242
304	404	276	237	289	367	246	251	338	303	218
298	322	256	277	263	264	253	296	302	336	246
267	260	216	307	299	278	311	286	276	295	293
268	216	158	238	303	302	197	241	182	246	238
213	177	246	201	266	157	364	223	250	239	312
408	326	195	194	372	449	357	192	242	471	157
294	264	399	214	288	289	245	243	344	257	368
264	300	350	387	286	318	371	407	267	166	246
247	310	142	185	320	223	208	282	326	245	363
249	161	217	211	406	267	357	344	274	315	142
291	172	336	287	264	299	261	294	279	299	362
180	199	186	348	233	366	262	225	175	295	271
161	319	318	149	298	227	308	222	313	233	341
267	322	298	179	343	225	277	245	296	192	295
279	172	188	251	311	260	264	165	277	320	358
329	298	334	325	210	337	336	256	359	320	244
217	25	231	305	256	389	265	315	382	352	304
227	225	306	238	252	301	204	233	188	266	292
211	216	235	304	344	268	382	292	144	279	216
316	265	95	303	295	214	275	278	295	295	286
244	232	343	337	299	379	305	351	342	284	

225

1200.0_1135EC03	223	156	999	274	255	210	192	189	127	207
	282	131	165	221	212	193	192	225	262	225
	205	186	31	168	250	164	194	173	211	236
	234	161	158	214	40	842	260	141	270	187
	278	243	0	258	30	213	237	189	190	210
	219	198	200	201	212	159	199	193	8	209
	223	99	204	185	206	185	199	194	278	229
	237	218	228	157	162	237	187	166	186	201
	180	140	134	3	146	284	194	157	188	140
	188	199	187	700	259	160	219	236	201	199
	0	118	64	55	230	225	123	159	143	161
	239	141	164	118	120	57	40	162	188	195
	147	171	263	145	184	210	714	139	340	19
	145	206	202	173	228	231	229	227	220	209
	230	106	114	170	168	220	165	144	126	188
	198	677	80	165	153	154	258	8	81	22
	23	41	69	0	621	53	237	113	174	616
	143	139	262	189	234	192	8	107	218	38
	128	3	217	215	150	208	0	1	166	106
	158	106	144	134	169	205	286	205	136	20
	34	58	178	55	131	1	269	144	80	210
	125	0	96	145	206	168	137	123	1	193
	118	139	174	0	49	4	110	196	1	11
	93	175	130	398	145	222	21	41	77	208
	165	210	30	0	60	9	195	15	157	174
	239	0	209	103	195	190	41	6	60	120
	0	144	0	0	208	14	9	226	12	126
	1	167	146	129	164	275	198	200	189	112
	61	0	2	227	128	29	157	25	144	233
	14	212	204	63	0	211	69	11	123	81
	2	109	203	94	252	2	213	52	165	224
	56	106	0	49	176	0	0	82	86	1
	186	45	184	239	82	129	152	135	47	95

226

1221.9_1185EK06	312	361	274	999	910	385	340	240	392	327
258	368	363	462	310	321	309	289	349	370	448
474	323	377	439	317	299	379	489	339	544	322
321	322	278	316	326	239	347	474	375	391	196
298	384	388	409	235	311	389	246	328	338	330
452	313	332	311	352	379	313	217	333	226	243
209	338	303	242	254	282	339	261	247	304	436
286	272	405	292	279	314	195	175	289	304	296
306	311	332	267	303	189	335	326	347	346	305
347	318	310	171	321	262	331	308	413	326	324
248	315	316	332	476	275	281	257	285	255	277
233	290	169	345	334	266	230	283	251	370	310
283	296	231	178	338	312	175	433	237	311	225
247	473	266	250	271	267	260	276	277	343	252
289	296	300	323	314	279	304	266	313	309	304
293	160	284	300	312	308	193	170	185	128	208
204	44	156	169	176	177	287	164	269	149	960
392	321	133	371	413	340	429	246	270	378	239
336	267	354	223	299	326	319	351	473	275	320
392	254	393	423	469	282	386	411	347	151	334
275	350	301	285	390	127	281	283	367	424	199
283	0	324	185	482	403	455	335	308	360	72
316	75	411	279	344	399	290	369	321	369	310
262	350	231	310	306	346	320	222	357	416	313
191	346	362	165	287	243	391	297	194	88	439
179	360	311	273	372	6	327	237	324	179	289
0	273	165	362	376	363	312	260	339	486	363
299	338	296	311	257	294	327	305	291	338	298
362	25	286	332	330	411	294	378	412	310	351
305	300	421	320	305	281	240	254	325	246	318
237	254	313	357	362	304	392	320	110	295	288
292	280	125	248	302	118	330	216	320	319	279
214	297	300	316	311	298	237	260	235	286	



227

1260.4_2011EC44	294	341	255	910	999	376	322	297	358	325
292	365	384	456	295	331	310	263	352	352	396
379	343	368	424	303	321	366	396	359	458	351
338	351	264	333	315	230	315	443	333	347	213
274	378	407	332	213	276	325	235	318	328	337
344	289	310	287	312	314	291	279	318	249	260
303	328	311	269	265	261	343	295	253	296	368
296	324	404	290	279	297	196	196	278	303	296
306	311	325	273	289	186	322	341	333	310	306
312	307	273	174	289	233	305	308	386	321	319
235	311	312	325	365	282	292	270	298	269	287
247	280	158	344	340	296	239	300	247	357	296
301	317	253	198	347	326	172	352	264	262	233
255	483	251	241	273	257	267	291	282	347	242
276	281	317	310	300	271	295	244	312	295	299
287	167	269	292	314	311	222	176	214	157	213
289	159	255	170	178	175	307	213	244	156	933
376	290	164	350	391	322	398	263	321	353	203
357	334	378	224	302	348	232	370	405	244	342
351	274	349	406	399	347	370	400	363	246	339
185	360	304	335	368	119	253	351	364	338	162
302	0	339	200	457	378	362	332	353	338	160
296	77	333	345	338	387	274	358	346	359	288
270	319	274	303	317	361	336	325	308	376	318
240	336	311	223	299	322	357	341	256	175	402
260	375	314	282	364	234	312	250	309	219	281
0	259	219	315	372	347	318	289	340	387	345
342	348	329	296	309	307	325	291	339	334	280
332	102	310	316	294	394	323	359	422	331	335
288	290	416	299	311	268	233	264	303	276	354
310	284	290	331	351	286	370	292	189	312	258
276	257	168	285	281	150	317	271	318	320	272
214	281	314	307	312	326	290	267	258	290	

228

1280.9_1164EK04	652	395	210	385	376	999	343	150	335	176
220	470	360	378	281	310	293	219	255	367	373
375	260	356	577	237	341	360	354	374	390	348
371	384	275	319	328	158	301	578	323	323	252
248	336	304	299	258	331	319	255	349	345	297
345	312	321	313	280	626	303	231	273	222	323
234	299	346	328	207	260	338	328	273	214	272
227	260	338	244	289	294	219	288	290	296	302
311	295	296	260	300	218	305	332	301	288	295
291	282	275	119	293	133	287	329	309	315	312
254	243	244	255	328	259	291	306	274	303	228
261	228	210	269	236	239	202	327	329	356	231
260	371	243	234	324	335	118	290	291	301	129
234	414	236	244	221	246	220	259	254	309	235
229	263	219	273	272	250	277	232	289	288	296
254	111	318	233	297	292	242	234	32	234	261
131	38	232	221	97	171	251	257	237	111	378
363	313	216	311	935	343	354	131	198	508	64
283	237	330	216	219	310	163	336	403	239	443
483	239	486	527	318	284	353	410	284	5	316
272	323	155	205	359	99	254	284	273	332	248
226	0	213	180	367	221	315	251	247	354	50
210	115	589	294	281	307	154	302	307	289	336
187	214	194	317	216	338	256	165	225	255	261
224	303	322	210	203	263	283	253	191	54	335
193	224	307	327	318	11	293	239	278	46	242
0	267	123	288	275	268	247	173	261	301	333
234	251	330	294	269	267	260	350	345	284	214
215	24	315	285	258	345	318	374	364	273	269
281	330	322	237	255	243	189	205	197	233	295
193	207	256	272	259	280	345	264	118	292	240
211	246	55	291	251	99	251	111	282	273	217
233	210	267	236	185	275	190	261	228	188	

229

1291.0_1185EK01	348	449	192	340	322	343	999	191	391	790
292	320	404	537	313	361	845	262	310	389	389
411	212	329	399	302	436	393	421	403	474	404
399	391	253	321	352	220	347	455	379	345	316
269	375	346	331	187	299	370	252	255	348	317
385	305	327	315	278	346	316	267	354	285	275
318	325	279	272	306	262	359	256	290	255	344
317	319	389	304	299	327	205	335	330	315	253
259	326	290	292	278	203	355	305	340	326	314
320	331	299	185	289	216	318	299	356	307	307
208	325	325	333	375	340	318	270	260	275	267
277	225	159	318	322	284	250	308	231	357	289
284	305	312	164	325	366	170	394	295	277	202
253	385	279	238	259	287	253	274	260	328	284
278	266	255	319	299	241	296	255	324	317	344
283	163	219	306	300	297	241	202	48	229	229
239	113	178	180	182	201	240	213	284	173	313
368	357	94	308	345	999	426	209	806	339	223
366	321	388	236	280	327	270	304	416	280	458
358	307	383	433	415	301	443	466	322	143	364
308	358	217	221	398	142	217	377	343	389	176
239	0	265	235	420	303	389	296	328	338	30
252	87	364	341	314	303	269	330	323	381	347
332	297	249	284	222	391	322	191	305	343	296
194	346	322	248	243	303	366	305	259	176	376
218	291	334	225	374	240	307	218	301	134	294
2	316	206	330	342	297	330	160	342	378	358
284	320	355	313	267	279	344	253	350	305	305
295	189	337	364	318	370	270	350	417	277	300
184	250	359	255	261	265	207	266	287	242	473
313	276	263	340	356	299	343	263	151	307	278
268	283	134	306	282	145	261	159	302	291	273
237	277	249	270	253	280	211	263	240	200	

230

1293.1_1164EK02	195	192	189	240	297	150	191	999	274	226
243	204	253	265	290	286	195	261	257	258	162
165	194	287	205	197	245	259	201	258	291	272
249	268	246	287	280	174	260	216	204	234	256
249	207	220	166	170	311	266	232	207	174	262
213	209	218	198	169	229	200	651	251	578	210
617	232	234	208	570	594	218	203	326	635	222
571	285	161	273	247	342	184	275	257	287	252
267	240	229	148	269	166	251	273	229	246	234
246	230	216	195	229	265	217	218	177	248	249
220	234	237	249	263	238	92	270	247	268	239
231	170	250	212	214	231	243	245	251	262	263
238	194	225	259	157	143	146	174	195	202	132
238	136	508	525	532	507	508	554	493	450	500
529	210	196	248	260	218	224	221	234	263	256
207	154	151	217	243	238	303	263	179	240	266
242	107	243	236	142	169	265	303	251	139	298
265	294	208	189	164	191	305	955	137	238	2
273	233	275	190	262	256	170	315	242	242	188
205	124	236	297	291	289	218	242	275	34	276
231	272	186	240	263	145	254	178	228	182	84
295	148	240	246	179	195	223	178	269	232	90
245	421	198	267	164	284	124	254	243	266	482
209	205	234	209	251	176	666	16	258	198	232
47	301	262	202	246	597	125	274	199	98	323
221	320	209	206	163	193	241	227	270	215	208
243	243	192	259	170	285	240	169	259	271	228
281	240	179	229	462	228	142	210	200	231	287
431	401	158	265	262	266	151	232	292	231	193
107	220	242	226	258	570	369	525	209	536	278
463	494	246	251	274	517	313	253	56	206	511
224	521	436	251	237	74	264	139	243	271	237
422	358	323	311	258	306	265	291	281	218	

231

1302.8_2011EC21	355	353	127	392	358	335	391	274	999	286
339	429	370	417	492	512	338	359	421	419	550
515	233	585	355	287	477	344	384	736	487	687
721	707	499	551	730	159	624	373	445	317	403
374	342	646	403	216	435	389	255	383	327	478
422	551	535	545	335	356	529	371	647	329	533
372	700	565	545	309	404	299	576	447	455	317
380	507	274	414	447	451	225	410	478	611	635
628	655	625	296	625	152	653	647	656	627	635
625	656	681	155	697	218	690	241	311	603	602
365	598	603	616	426	373	284	683	322	681	498
409	243	333	575	540	391	325	233	394	341	445
357	329	285	367	292	181	156	382	289	274	164
360	198	384	448	407	389	401	438	393	471	358
430	499	400	555	567	418	554	468	623	546	653
418	128	303	527	520	538	239	437	172	401	452
311	341	402	442	143	220	312	432	435	168	417
372	524	181	206	310	391	974	246	244	489	24
300	454	547	232	353	366	504	472	519	330	289
313	136	302	428	347	453	289	364	485	188	506
277	729	99	239	417	110	351	283	582	413	234
404	1	445	272	316	282	455	238	664	582	45
199	175	379	460	252	633	158	364	604	695	556
363	375	269	276	442	247	461	164	486	303	515
145	582	619	327	486	392	217	449	203	41	597
381	581	568	326	226	271	629	365	585	189	495
284	526	137	582	267	527	629	291	663	424	571
587	599	263	540	385	277	143	315	325	532	487
309	93	330	565	602	676	396	471	619	313	278
226	300	574	516	555	522	258	357	435	421	675
404	402	468	600	563	460	528	524	219	402	393
422	397	118	518	500	142	512	84	510	545	533
308	377	260	279	241	351	244	334	285	278	

232

1315.1_1164EK04	191	235	207	327	325	176	790	226	286	999
264	212	262	353	275	255	806	231	300	313	288
330	154	197	339	302	351	275	352	220	454	249
237	224	181	251	221	217	262	381	307	262	286
266	350	204	306	91	287	359	160	200	245	226
339	219	253	227	240	300	234	274	247	217	162
316	237	194	153	275	237	264	141	188	233	317
234	243	303	241	185	264	129	233	250	246	247
245	208	235	229	256	163	292	232	286	252	209
236	273	249	173	238	217	237	236	302	231	232
128	211	211	231	369	283	187	221	156	246	229
213	208	119	292	254	209	184	247	155	277	215
166	186	304	131	237	281	154	357	226	257	175
183	293	233	219	218	238	204	232	221	267	249
230	232	181	281	248	251	247	233	243	231	250
244	143	174	249	278	236	214	149	98	154	161
124	23	126	124	179	220	224	163	270	147	313
277	315	134	296	191	790	313	321	970	190	249
261	207	256	204	278	278	230	217	343	261	333
374	210	234	300	394	250	341	421	276	138	261
219	316	205	200	333	164	235	344	239	332	20
238	0	271	180	312	288	356	269	215	290	50
204	44	324	260	296	275	230	275	231	264	320
209	249	177	209	314	251	324	191	308	308	291
131	341	297	104	217	287	311	245	188	145	339
221	296	312	181	283	6	226	136	259	106	229
0	246	1	263	275	264	246	145	269	382	271
220	270	233	224	225	198	266	171	294	220	229
207	131	267	292	215	315	260	317	376	211	239
183	170	326	228	190	273	133	191	263	153	494
291	204	251	309	329	250	303	235	121	238	256
259	225	57	220	251	2	245	76	292	244	236
253	295	238	228	190	239	158	225	195	151	

233

1318.8_1185EK05	283	304	282	258	292	220	292	243	339	264
999	245	282	508	314	350	249	282	264	259	242
283	267	294	306	328	309	316	240	328	304	339
322	319	244	376	276	346	366	337	253	298	305
279	368	366	224	212	254	259	208	193	290	299
229	259	281	266	235	305	264	286	252	289	245
282	273	304	241	313	233	265	267	237	281	301
249	270	601	220	232	307	195	211	257	277	268
263	268	275	219	272	207	285	295	293	250	277
252	274	232	315	230	280	244	197	301	275	273
215	256	254	261	202	276	186	297	270	296	312
228	180	198	281	282	289	257	186	196	340	227
251	272	277	181	227	329	294	284	199	149	270
239	334	243	234	227	253	203	229	223	323	217
230	238	252	286	269	234	273	215	260	256	288
244	294	237	245	286	254	205	207	155	132	190
16	154	186	240	303	217	323	146	221	274	290
333	256	178	261	217	292	368	300	266	272	944
309	348	276	331	328	309	199	371	300	295	321
297	237	240	324	263	315	381	451	329	183	383
213	336	266	326	306	134	238	282	341	218	153
315	0	316	639	647	288	252	352	330	317	140
306	266	298	289	324	341	191	300	311	285	294
262	280	331	324	446	395	309	244	277	309	296
221	363	317	231	284	322	577	301	287	372	347
271	319	242	233	266	61	249	306	283	218	264
0	244	264	279	273	325	273	178	301	243	310
297	334	342	292	240	285	320	266	287	296	243
276	73	252	315	236	342	235	331	356	297	315
122	273	364	320	287	233	232	223	262	205	402
253	243	252	301	321	257	355	263	129	319	257
270	262	197	289	244	251	269	242	286	262	248
231	229	320	334	297	326	294	297	276	277	

234

1318.9_1164EK04	377	390	131	368	365	470	320	204	429	212
245	999	320	349	346	319	320	256	306	330	391
580	282	566	346	222	322	358	422	453	397	470
467	464	287	301	360	121	351	377	385	345	260
245	383	445	307	306	246	329	244	424	278	424
367	293	299	291	340	387	283	254	327	239	503
239	353	490	518	261	242	292	484	259	284	340
283	336	358	285	314	302	210	235	258	305	300
310	310	310	285	313	209	345	382	355	364	299
357	315	327	111	341	181	308	298	322	391	385
269	300	300	305	377	312	291	351	298	347	307
301	263	281	350	324	323	246	284	274	303	256
284	294	268	322	368	280	104	280	348	355	246
269	268	271	254	284	260	242	248	247	291	253
256	285	196	377	370	241	337	282	349	355	346
266	94	404	328	336	347	214	296	106	296	290
262	194	260	302	91	219	255	301	282	91	339
424	337	101	148	479	320	434	185	10	940	5
198	273	398	213	313	275	296	418	577	236	417
259	135	464	524	304	285	263	400	286	334	324
288	327	144	184	362	76	229	251	395	324	335
271	0	243	152	347	284	371	300	397	326	154
196	111	394	377	209	323	109	310	451	372	333
196	223	235	286	293	345	252	0	310	291	283
154	315	388	69	318	249	262	261	123	130	400
235	325	338	402	304	116	321	275	293	34	369
5	281	171	268	295	225	324	155	361	366	379
314	375	282	357	254	338	238	391	380	380	206
330	21	285	314	305	380	188	289	375	382	314
304	389	315	284	340	265	165	227	221	195	373
237	210	264	320	289	234	421	325	116	283	233
269	269	127	376	311	146	336	57	338	327	337
200	234	244	249	219	307	228	275	267	254	



235

1326.9_1185EK07	360	356	165	363	384	360	404	253	370	262
	282	320	999	405	333	390	376	289	340	397
	379	169	333	602	314	336	807	370	385	370
	409	404	333	354	318	171	300	465	421	283
	293	679	382	279	166	377	393	250	352	317
	314	318	305	300	319	349	311	355	276	309
	334	303	301	307	302	288	693	316	336	272
	282	319	482	231	301	303	194	344	304	280
	285	302	311	387	302	227	320	331	325	297
	275	310	310	180	302	150	307	753	537	289
	213	259	260	269	352	304	222	330	263	277
	272	203	146	285	278	293	263	737	320	252
	273	309	296	181	262	468	177	279	274	151
	266	469	263	267	300	310	285	321	319	279
	264	271	239	304	290	273	312	254	296	307
	272	164	180	249	318	309	190	270	106	304
	292	232	259	283	150	217	266	260	254	360
	368	316	115	727	338	404	387	262	252	108
	929	363	398	250	294	424	249	332	370	305
	378	503	364	438	272	355	394	405	309	346
	260	316	195	295	426	174	278	507	306	144
	274	0	269	241	302	377	294	340	330	19
	134	170	379	361	307	284	303	330	385	355
	222	304	384	284	226	564	313	383	291	339
	535	292	338	242	240	305	407	271	207	351
	201	316	354	200	554	358	309	228	292	306
	1	282	201	318	480	311	269	221	282	334
	277	324	621	322	319	217	367	218	702	233
	264	213	751	301	297	423	519	557	448	246
	208	208	422	264	264	270	163	281	206	355
	305	272	245	341	261	340	363	250	102	258
	261	265	62	335	257	231	305	96	305	254
	228	224	236	231	226	271	214	253	241	191

236

1334.7_1344EC21	448	547	221	462	456	378	537	265	417	353
508	349	405	999	447	452	407	308	421	418	441
452	287	416	436	357	396	426	413	438	474	401
446	424	334	407	354	198	360	412	585	349	401
393	435	425	363	202	388	420	298	333	365	402
387	363	365	367	369	418	365	345	315	324	363
317	351	348	369	316	312	362	349	356	282	411
313	312	519	320	354	412	216	379	351	377	364
383	381	378	302	395	213	371	326	376	356	388
369	376	367	170	369	186	371	287	460	367	369
294	294	300	303	431	336	283	398	268	399	327
318	296	251	357	329	318	196	270	334	423	282
267	368	351	292	380	337	178	357	268	238	247
247	386	297	300	302	310	297	334	331	360	302
288	293	336	331	322	352	329	249	298	298	319
378	160	197	279	313	299	239	296	80	318	303
251	248	296	294	170	214	313	313	249	158	433
427	399	90	263	336	537	422	211	306	420	362
340	420	398	257	358	388	296	370	427	390	333
364	263	358	397	364	404	487	453	438	216	399
299	408	227	281	549	82	362	328	408	386	203
332	0	322	426	584	359	382	389	360	406	58
253	188	415	384	344	386	241	400	341	359	400
211	344	256	296	332	433	306	205	384	417	353
218	387	437	268	245	320	412	332	203	157	434
255	302	352	211	382	254	373	221	361	134	323
0	277	132	271	384	344	304	187	331	397	400
283	386	370	352	242	273	330	247	349	321	316
276	54	350	355	293	434	270	420	423	274	310
157	237	440	322	296	341	224	267	325	295	436
231	278	361	393	419	311	378	311	135	325	316
307	298	132	289	290	97	269	155	313	277	273
271	242	292	275	268	314	252	258	216	232	

1336.4_2011EC31	349	339	212	310	295	281	313	290	492	275
314	346	333	447	999	674	285	627	659	320	304
335	290	374	270	303	469	335	262	461	322	511
492	493	575	594	483	221	438	329	329	302	339
330	319	505	268	214	418	344	239	238	240	505
289	334	329	330	282	259	329	286	350	278	312
248	454	354	316	249	311	231	343	504	322	354
327	379	331	493	439	459	174	395	465	431	370
376	434	401	349	380	250	416	389	409	417	425
401	423	382	194	398	194	416	181	293	416	410
229	367	366	359	260	326	157	536	251	537	446
340	208	183	419	362	401	170	226	312	313	382
260	257	289	222	301	172	197	317	278	224	237
244	238	291	315	301	292	295	317	306	377	339
361	330	359	351	333	323	334	282	371	309	378
356	193	219	312	326	310	227	377	124	364	372
303	290	339	401	195	190	306	309	284	192	291
532	606	212	215	261	313	525	251	190	411	160
319	632	424	384	716	339	376	491	358	339	230
323	171	299	333	220	581	348	273	630	266	573
139	512	191	319	353	118	319	227	514	281	221
474	0	445	310	346	286	316	314	422	383	82
260	137	272	496	363	428	175	333	455	415	369
223	419	328	272	344	254	347	151	403	353	466
114	434	372	278	323	359	209	485	208	199	431
333	403	384	209	204	308	383	214	345	202	314
0	364	181	393	245	519	382	253	419	285	370
343	470	191	345	354	233	200	257	202	394	440
302	123	355	369	365	407	160	438	405	259	234
184	242	406	423	369	356	301	344	349	329	429
353	367	354	367	380	323	444	324	254	400	315
309	306	204	363	318	152	303	130	343	353	294
234	304	309	327	297	355	276	327	282	226	

1346.0_2011EC29	367	348	193	321	331	310	361	286	512	255
350	319	390	452	674	999	294	369	741	371	393
402	281	446	309	375	592	390	341	535	394	511
495	512	578	513	450	216	426	329	396	321	377
327	361	525	346	257	477	418	215	293	336	435
336	392	390	393	423	344	390	275	421	310	347
272	491	366	353	259	403	324	350	438	424	319
365	379	340	374	461	480	208	446	450	429	406
453	489	430	412	445	209	456	414	470	394	460
394	495	481	159	453	164	491	226	312	426	425
262	387	387	370	290	351	232	483	248	488	455
363	260	208	393	380	383	193	259	326	371	389
253	272	276	263	333	218	178	372	254	225	217
222	245	346	395	359	339	339	346	324	370	361
355	400	304	424	399	381	405	341	377	388	438
367	166	256	368	410	379	157	386	167	314	368
293	375	314	310	185	221	287	349	322	126	325
522	639	171	224	299	361	522	283	192	401	203
347	950	456	355	469	370	400	438	388	319	276
352	181	310	357	255	705	344	321	630	260	523
256	485	164	291	391	69	301	253	454	369	243
420	0	445	339	315	306	365	390	462	435	0
269	126	343	451	305	478	240	353	485	465	498
237	461	338	326	359	288	421	168	394	315	365
155	435	522	286	334	369	216	504	248	146	445
366	397	373	262	232	355	433	217	371	139	389
0	398	227	417	272	549	423	293	432	366	429
371	512	269	364	342	281	197	289	259	403	435
371	192	380	380	395	467	207	543	459	292	253
182	282	456	430	359	483	274	378	345	362	512
338	384	370	396	383	373	465	374	168	417	414
355	379	171	456	383	189	385	190	414	393	362
317	365	266	314	283	330	287	302	261	306	

1351.6_1344EC23	306	340	192	309	310	293	845	195	338	806
249	320	376	407	285	294	999	248	315	379	380
386	197	317	389	341	422	372	368	347	442	339
334	331	273	303	280	162	280	413	339	336	295
307	359	324	324	146	267	369	205	223	319	292
364	298	323	307	286	330	310	241	295	255	278
311	272	266	272	281	234	341	239	260	251	354
288	278	363	282	246	304	191	292	288	309	284
290	319	303	340	292	213	335	274	336	269	314
254	326	289	159	276	190	302	286	344	253	254
157	273	274	285	341	301	269	241	230	260	260
230	183	177	300	268	256	199	272	179	364	258
239	277	282	163	327	328	165	368	247	243	193
187	344	250	234	235	255	211	227	215	314	270
258	245	255	279	251	232	270	235	283	262	289
298	161	215	273	283	251	229	191	90	226	204
188	22	167	187	176	202	245	192	238	147	284
357	357	151	374	312	845	381	226	858	328	197
329	259	357	211	301	334	202	299	408	254	438
348	254	335	386	395	298	396	450	361	152	317
300	325	323	229	393	184	277	423	331	376	110
247	0	309	253	378	333	361	292	296	327	60
218	105	345	374	297	287	253	346	312	307	304
262	328	255	268	272	373	299	173	328	358	291
197	346	257	254	266	291	330	357	207	172	367
233	324	309	224	348	198	324	225	307	221	239
0	300	206	291	353	329	278	200	282	371	320
272	295	303	274	242	244	297	240	336	266	253
317	222	350	334	294	319	288	355	386	252	285
195	240	352	275	243	256	160	247	289	217	460
304	275	258	313	336	260	307	241	107	285	231
248	229	146	277	260	131	252	141	276	276	233
205	263	261	256	257	269	212	245	230	208	

1372.0_1288EC46	270	243	225	289	263	219	262	261	359	231
282	256	289	308	627	369	248	999	441	257	240
267	283	265	216	253	328	249	237	308	284	330
327	316	362	507	367	274	396	290	250	234	271
272	292	386	241	186	359	364	216	219	221	318
256	344	327	328	222	228	329	344	329	304	283
323	336	335	287	286	342	192	320	347	252	380
307	276	263	482	245	401	184	477	379	344	306
330	323	312	203	310	237	339	360	340	442	332
446	327	309	247	339	196	316	180	254	442	445
226	284	286	317	260	357	170	363	228	363	396
372	251	208	367	331	379	180	210	259	327	338
241	211	301	241	339	197	239	333	253	190	288
218	209	271	328	282	286	266	302	309	353	309
350	362	409	367	359	422	353	320	355	330	362
456	247	225	350	352	341	212	313	147	313	345
266	215	327	264	230	242	288	297	330	243	267
349	344	207	197	209	262	367	260	169	274	227
295	340	289	293	887	268	263	439	307	287	237
294	197	270	263	224	358	309	254	425	249	510
161	421	198	239	246	105	275	209	290	276	136
377	0	324	230	289	342	247	266	280	350	97
249	180	240	288	349	383	226	374	418	360	357
210	294	231	284	258	253	301	191	408	407	332
149	344	369	296	280	308	205	302	195	212	398
237	341	373	233	204	248	357	236	312	153	340
0	316	159	277	231	443	310	211	305	286	405
291	366	201	310	322	261	212	280	223	276	340
288	59	244	373	302	295	164	299	297	276	250
191	278	332	350	302	334	208	260	375	285	336
265	317	432	334	335	281	350	380	332	362	304
313	318	169	271	367	137	272	149	351	332	321
283	297	314	350	298	320	214	312	262	246	

1373.5_1164CC54	366	315	262	349	352	255	310	257	421	300
264	306	340	421	659	741	315	441	999	337	373
301	157	314	249	309	515	323	316	408	286	463
418	492	530	484	356	259	445	253	338	309	347
396	349	481	317	240	374	304	226	304	260	452
293	341	326	330	310	294	326	281	339	219	294
227	389	307	298	196	346	318	285	630	348	311
398	413	296	432	464	467	200	341	427	381	398
384	404	420	363	407	145	400	401	406	416	388
415	396	410	271	426	223	430	163	273	436	436
228	327	310	342	314	339	149	503	169	486	392
344	233	122	452	430	376	104	152	289	281	405
220	228	249	244	272	123	253	285	277	281	265
216	162	293	320	296	291	293	300	290	310	353
408	361	370	342	345	299	339	310	335	322	351
344	302	141	323	327	297	215	361	135	299	320
273	340	303	369	269	83	249	323	280	270	297
508	689	92	157	253	310	458	170	223	350	205
362	708	395	346	489	362	432	375	323	183	168
354	85	280	325	3	641	306	237	597	168	498
125	456	118	254	318	0	373	252	427	355	247
481	0	433	306	283	255	331	324	412	350	80
157	313	309	459	313	444	219	267	437	390	320
139	437	311	316	307	247	319	69	399	303	415
131	410	427	241	310	450	107	425	118	267	364
330	393	279	155	218	278	408	159	311	44	212
0	302	0	368	264	497	360	302	375	367	360
304	519	202	294	339	216	208	226	225	336	460
120	138	361	359	358	426	2	493	431	227	204
128	219	377	378	323	396	263	318	312	320	425
340	374	380	347	363	273	408	281	181	418	342
290	266	1	368	303	38	234	98	290	362	323
281	304	294	275	247	264	223	250	207	195	

1379.5_1185EK02	402	403	225	370	352	367	389	258	419	313
259	330	448	418	320	371	379	257	337	999	566
423	253	369	476	305	402	463	405	399	405	412
400	419	401	401	394	227	407	401	514	409	321
264	410	409	342	227	319	386	278	391	361	429
355	339	355	358	384	514	348	303	357	299	336
318	352	321	342	308	312	346	326	336	282	360
320	390	364	329	318	328	275	318	347	351	313
329	375	340	709	348	208	367	401	373	361	358
357	366	377	275	375	247	372	353	340	385	373
289	337	342	352	363	318	316	308	307	293	349
286	246	195	325	352	338	326	338	352	459	330
332	364	266	231	403	406	258	392	294	306	236
324	342	315	294	296	296	302	303	315	351	301
314	288	292	369	348	326	360	314	328	331	349
267	262	209	336	366	363	249	306	171	303	312
301	282	305	300	306	273	352	287	265	262	365
476	327	147	376	376	389	408	263	312	372	100
382	386	438	321	302	940	340	371	414	209	393
467	293	346	424	341	365	401	408	389	165	414
396	377	257	544	519	180	269	299	360	379	230
341	134	335	262	358	331	350	390	419	362	84
279	160	533	382	293	383	227	381	367	378	380
279	297	268	327	325	364	313	327	330	380	308
243	396	348	269	356	366	353	292	339	177	460
297	374	392	222	361	282	338	319	337	193	361
207	279	234	306	329	362	340	223	351	368	392
385	364	329	384	306	326	326	276	374	427	330
294	215	335	377	332	390	309	360	438	336	338
271	275	371	360	345	345	254	326	274	297	377
364	276	333	392	372	344	421	338	189	355	361
313	295	169	373	330	277	344	261	369	372	368
280	293	345	358	322	367	300	366	362	271	



1380.3_1164EK04	411	351	167	448	396	373	389	162	550	288
242	391	397	441	304	393	380	240	373	566	999
473	160	369	484	267	351	414	485	426	464	380
425	409	351	410	454	142	427	364	472	326	242
263	367	343	537	141	370	422	249	246	370	356
499	302	324	328	290	499	309	195	381	223	363
215	381	333	359	208	244	336	343	312	251	396
259	652	313	293	282	370	221	247	370	338	320
328	337	326	439	348	188	379	561	378	393	335
404	347	370	109	378	143	365	327	384	424	406
244	343	344	360	528	292	207	327	264	323	277
250	198	172	278	307	252	263	293	324	393	316
273	277	248	202	276	301	110	430	330	370	103
271	361	283	300	258	285	280	301	265	315	251
292	298	234	435	456	243	403	309	421	431	413
234	122	195	390	422	434	175	256	16	255	262
228	252	239	261	135	107	275	227	289	121	444
431	354	123	324	378	389	543	155	293	400	142
362	365	350	199	288	500	817	320	488	268	267
434	278	334	417	377	313	323	420	369	185	348
250	417	223	308	450	0	250	233	310	562	198
237	0	252	236	412	379	521	269	522	356	185
189	43	531	336	286	348	206	365	350	423	409
250	293	261	243	247	330	268	239	326	381	283
256	320	291	238	490	333	355	299	190	111	448
197	517	275	216	307	159	328	502	318	165	229
203	288	190	365	333	432	367	235	380	556	408
515	339	319	565	303	197	287	239	341	580	328
288	213	312	332	346	406	285	327	343	202	256
234	235	374	331	520	334	203	290	278	239	269
377	257	294	312	332	322	352	315	104	273	246
286	315	72	461	312	160	455	40	417	419	500
217	265	209	255	184	263	188	264	273	158	

1402.5_1164EK04	341	370	205	474	379	375	411	165	515	330
283	580	379	452	335	402	386	267	301	423	473
999	235	651	426	286	397	432	539	407	645	427
422	398	352	402	454	188	419	429	482	480	333
285	417	505	507	210	365	404	297	362	381	441
490	403	396	389	529	406	380	309	457	274	481
316	471	490	486	297	348	365	491	305	351	398
303	307	371	350	364	393	270	298	352	445	424
431	433	437	331	425	215	434	405	449	465	441
471	421	404	150	434	230	405	344	389	462	464
321	390	386	431	582	367	289	328	331	326	382
348	327	375	454	429	329	329	287	275	405	348
360	327	282	369	448	359	153	581	372	463	198
325	355	342	359	357	340	330	377	322	383	355
326	365	303	447	442	313	428	376	426	420	439
314	145	354	383	436	434	260	333	132	345	345
310	124	330	321	153	335	341	426	356	136	427
376	333	171	335	374	411	538	191	325	606	152
339	347	372	221	272	342	362	404	948	289	374
354	256	414	477	559	297	389	454	321	85	372
376	393	203	230	425	169	214	280	484	520	184
267	0	305	221	411	370	480	304	399	461	46
283	90	471	371	318	452	218	440	384	482	405
278	263	267	296	300	359	287	241	393	388	385
253	359	471	243	368	315	336	303	232	96	533
226	365	431	345	315	175	432	347	379	142	392
255	317	192	361	385	365	411	180	429	568	479
377	465	289	430	286	357	305	368	358	442	349
419	195	327	416	372	441	344	385	457	366	384
394	357	422	427	427	371	235	293	324	242	395
310	225	386	403	402	330	480	429	149	329	315
362	353	89	357	402	121	382	215	415	411	404
289	286	287	315	294	328	275	304	279	283	

1402.9_1344EC19	242	241	186	323	343	260	212	194	233	154
267	282	169	287	290	281	197	283	157	253	160
235	999	282	199	198	303	225	247	251	245	232
262	238	338	279	274	261	297	309	209	206	260
211	261	262	216	248	220	210	214	244	210	267
214	236	241	248	169	268	236	220	229	224	296
217	252	274	293	211	264	207	277	235	255	270
309	265	251	242	230	288	199	289	274	247	250
252	259	256	120	242	179	259	260	254	266	251
268	258	242	235	230	176	237	187	228	257	260
223	216	214	229	201	289	256	244	255	246	261
250	269	253	255	241	255	214	167	215	297	224
248	237	199	263	165	248	221	161	283	236	335
220	293	237	238	233	229	219	247	221	256	253
236	242	220	247	242	261	243	232	245	222	239
249	226	365	237	266	243	245	245	122	258	250
225	145	267	224	262	220	296	273	252	255	308
288	215	139	139	239	212	240	175	154	303	193
132	179	238	245	224	186	113	305	260	199	306
185	135	257	288	217	193	295	342	236	74	249
166	264	188	130	182	25	203	203	261	207	270
251	0	282	164	301	196	205	187	174	265	37
249	91	274	135	214	240	192	232	163	223	270
170	110	144	354	127	234	245	79	217	253	163
154	273	259	153	147	217	234	192	180	198	267
173	141	301	364	212	187	241	156	229	143	291
0	231	176	180	210	167	225	130	210	192	254
203	225	191	207	155	375	168	379	165	195	217
200	51	153	262	177	224	186	233	244	379	350
253	381	252	235	201	226	192	178	167	226	204
162	153	265	222	248	208	328	265	44	246	243
180	239	7	150	251	89	179	173	251	187	228
239	140	337	404	336	309	242	288	306	357	

1412.3_1344EC09	387	347	31	377	368	356	329	287	585	197
294	566	333	416	374	446	317	265	314	369	369
651	282	999	361	264	460	386	385	503	418	514
490	490	395	454	530	35	467	368	433	332	308
372	368	505	351	228	402	340	306	413	316	446
421	409	415	425	367	306	414	329	468	311	639
327	517	621	653	302	383	316	646	309	381	340
330	331	281	344	394	409	298	337	356	477	477
488	491	473	292	490	184	476	450	490	491	479
490	494	484	125	497	223	491	282	355	510	508
411	429	433	464	393	354	278	460	362	459	428
351	299	372	477	442	357	293	261	350	365	366
382	391	297	403	370	195	146	392	300	309	219
330	232	359	366	375	360	349	394	353	414	364
358	427	307	453	447	392	445	420	474	424	500
362	27	411	423	429	426	222	396	175	394	410
368	285	379	406	46	371	311	490	373	26	380
356	314	166	256	317	329	584	222	189	575	136
254	390	385	224	299	346	336	539	653	271	331
379	149	346	464	326	364	302	363	351	223	430
306	523	150	203	388	3	339	301	466	366	218
355	1	363	243	322	269	433	297	452	474	25
260	128	326	458	337	493	178	363	491	506	449
188	311	245	280	319	260	336	120	423	318	379
156	438	541	231	446	269	202	380	236	0	526
278	396	442	412	266	244	479	287	435	148	436
275	304	143	377	275	342	482	186	484	406	476
423	496	253	414	312	389	156	404	308	408	397
338	52	314	397	401	488	250	385	471	398	389
300	382	445	361	424	398	254	316	305	329	519
300	326	388	423	421	347	486	445	171	294	355
382	364	113	361	447	82	386	149	423	413	408
263	302	266	302	292	357	305	330	278	327	

1412.9_1164EK04	462	322	168	439	424	577	399	205	355	339
306	346	602	436	270	309	389	216	249	476	484
426	199	361	999	293	322	503	436	357	456	300
359	329	269	326	290	147	289	603	420	348	268
263	566	311	378	174	348	408	276	367	587	297
360	309	313	299	353	586	306	319	261	287	337
348	303	324	335	299	253	582	319	252	226	355
243	238	483	237	282	299	208	339	251	310	298
296	309	311	362	332	210	279	279	290	286	301
287	274	257	164	261	172	261	571	499	287	294
234	238	239	243	396	275	254	283	227	280	223
227	252	225	269	260	241	202	559	353	384	219
234	307	314	228	338	465	163	356	297	299	124
233	537	234	273	246	266	244	271	266	320	253
213	236	230	259	240	251	267	209	287	274	292
282	121	292	216	268	237	261	249	130	259	261
157	114	266	254	117	174	265	274	231	110	397
391	337	175	604	559	399	372	130	297	390	221
531	268	280	173	243	391	212	357	411	195	408
447	404	393	415	371	269	440	545	275	179	317
317	295	182	312	412	59	252	510	282	472	142
215	0	216	279	386	326	334	344	255	353	42
200	135	562	280	362	280	231	322	314	289	331
199	256	333	305	255	574	238	344	250	339	265
443	301	315	150	192	271	453	258	138	141	367
184	208	285	282	516	148	297	182	286	101	292
0	221	137	256	464	254	223	212	254	357	312
220	271	612	280	260	272	325	295	590	255	209
255	28	584	270	265	414	490	464	470	272	257
250	288	484	243	234	269	183	210	226	235	348
232	218	246	316	298	296	362	231	158	266	224
203	261	71	266	240	189	239	138	267	240	217
239	217	229	227	188	243	104	238	249	202	

1419.2_1135EC00	253	256	250	317	303	237	302	197	287	302
328	222	314	357	303	375	341	253	309	305	267
286	198	264	293	999	318	325	239	271	299	266
285	292	262	252	250	282	331	259	290	275	366
327	301	299	260	220	325	308	194	267	295	261
261	265	264	273	287	248	257	279	218	290	259
265	226	259	264	281	309	288	253	277	273	278
268	281	315	257	219	333	173	233	454	271	262
265	262	248	265	259	197	273	245	276	251	241
267	272	249	302	260	193	266	244	309	263	269
272	263	269	281	234	292	207	303	226	293	226
261	242	184	223	201	236	144	234	211	277	203
226	241	236	227	246	275	299	266	267	220	256
209	289	279	311	299	300	272	287	253	301	279
309	251	248	282	270	244	277	227	257	282	273
284	288	208	249	270	254	190	424	103	416	426
313	252	402	390	295	190	304	264	253	278	297
311	318	164	192	248	302	306	171	237	275	193
266	275	237	482	318	335	268	292	299	218	265
277	219	294	305	260	347	340	291	264	174	261
266	271	206	140	282	78	315	305	277	244	230
269	106	281	287	299	302	276	296	202	289	24
199	110	269	223	235	274	229	277	264	251	306
179	207	432	316	199	282	245	254	198	294	242
180	323	306	185	240	280	246	292	245	257	258
314	228	233	200	247	234	276	173	243	135	186
0	262	126	208	288	235	284	269	233	240	301
231	253	276	242	284	243	208	222	269	267	210
225	20	253	266	224	275	186	293	317	278	254
145	229	320	281	255	266	218	229	242	176	280
192	291	232	273	283	249	335	228	122	268	244
218	268	112	271	256	56	180	237	264	239	209
245	267	344	343	299	301	352	328	281	246	

1428.7_1344EC11	365	353	164	299	321	341	436	245	477	351
309	322	336	396	469	592	422	328	515	402	351
397	303	460	322	318	999	361	318	467	353	420
476	473	462	471	435	171	433	445	383	318	375
300	310	444	278	219	458	374	269	362	358	397
293	363	376	379	360	337	377	329	398	297	400
322	445	408	399	289	326	322	380	424	364	323
357	450	295	398	368	481	192	383	389	424	387
387	420	397	328	426	154	442	476	429	446	411
448	436	429	153	450	172	460	229	287	507	501
268	387	383	373	288	354	299	437	288	449	402
339	294	219	398	392	335	229	227	341	402	349
307	319	274	249	340	259	152	292	329	316	264
268	249	349	386	360	349	345	380	322	374	387
316	357	373	455	452	323	422	362	422	422	429
366	142	274	401	420	414	221	293	88	287	306
282	298	298	278	166	232	321	358	363	181	285
481	499	186	201	328	436	471	245	327	386	141
267	552	429	339	401	318	355	480	417	352	351
417	116	340	412	245	468	326	322	460	188	482
264	485	101	248	391	14	263	335	434	295	211
371	0	477	335	309	225	309	315	443	424	65
259	111	346	368	313	449	229	396	404	439	472
226	398	304	361	264	287	373	98	347	313	378
150	445	414	367	388	384	219	418	197	49	473
314	443	425	286	250	308	390	307	345	49	383
21	392	164	387	262	493	395	220	418	311	436
429	446	320	428	308	303	210	299	317	425	415
369	137	300	428	371	450	169	424	469	322	314
225	302	439	360	432	383	241	322	375	335	498
400	322	366	396	394	362	466	398	209	406	337
350	342	180	401	383	110	392	209	437	389	435
281	329	315	324	265	345	290	351	289	257	

1440.4_1185EK03	386	417	194	379	366	360	393	259	344	275
316	358	807	426	335	390	372	249	323	463	414
432	225	386	503	325	361	999	403	404	380	377
416	435	375	378	328	201	324	425	486	416	298
310	608	453	309	185	348	391	288	364	594	359
370	350	355	357	375	365	366	343	294	282	347
349	316	356	344	301	306	597	348	302	309	315
298	345	513	263	314	355	191	354	299	333	310
320	321	340	411	345	242	330	377	348	325	321
334	350	353	200	343	172	345	592	464	350	347
301	272	271	284	387	298	297	322	274	314	314
307	235	203	306	324	309	267	561	342	381	262
303	372	272	249	329	417	196	325	314	265	172
294	444	258	305	327	313	287	333	315	357	337
253	287	264	342	332	331	363	262	307	368	318
315	185	191	284	363	350	206	299	134	239	309
290	252	269	285	180	217	298	297	275	179	354
423	311	139	610	347	393	365	239	204	407	172
781	334	390	300	261	399	299	361	408	295	344
405	440	426	469	294	370	389	406	379	193	383
316	370	193	243	489	160	315	461	341	330	206
275	0	293	295	366	376	386	407	316	365	105
174	210	394	370	331	327	228	342	350	336	373
242	278	405	312	335	528	330	302	279	321	329
459	337	368	239	275	329	400	304	232	85	379
264	316	385	214	484	302	345	284	317	120	309
3	322	199	323	436	290	300	254	301	346	376
283	358	541	329	275	231	364	210	599	322	290
254	36	585	345	287	473	486	513	455	232	277
194	192	426	352	311	292	228	281	288	280	361
331	271	293	362	307	338	376	265	122	293	279
249	302	84	334	276	182	346	155	364	368	284
239	258	250	247	196	272	213	259	243	216	



1441.4_1344EC30	326	376	173	489	396	354	421	201	384	352
240	422	370	413	262	341	368	237	316	405	485
539	247	385	436	239	318	403	999	347	638	307
334	343	267	295	358	147	337	395	476	372	228
258	388	376	569	234	326	356	268	298	401	306
635	313	329	312	428	369	309	244	354	241	323
238	344	333	323	246	282	388	319	251	302	319
281	232	376	230	321	296	220	259	278	311	323
334	318	324	346	349	282	306	315	326	358	291
364	290	285	118	300	202	291	353	400	341	344
235	308	307	331	709	300	232	235	302	232	262
257	251	201	295	304	250	282	350	314	370	264
318	308	305	250	368	329	120	575	285	370	233
314	331	264	258	293	287	258	290	277	342	253
253	290	220	297	298	301	301	239	310	322	319
303	122	186	267	319	317	235	227	99	236	234
320	223	222	228	128	242	306	262	273	132	470
422	345	143	376	361	421	401	220	263	477	96
382	289	311	230	248	336	419	302	569	204	304
336	319	355	394	569	309	371	451	268	275	309
283	322	257	216	409	118	226	288	333	624	220
210	0	237	222	439	312	636	339	276	345	214
232	91	449	289	292	377	190	378	272	360	324
152	234	216	287	247	356	277	225	374	322	272
265	300	356	234	244	292	349	251	254	96	405
184	231	327	209	356	226	330	217	327	114	288
1	232	240	270	380	278	319	254	341	690	377
225	322	341	320	272	246	254	238	326	314	293
339	26	308	334	304	354	285	361	365	271	267
281	228	324	306	244	285	185	243	291	199	257
246	214	315	340	276	309	340	289	139	273	252
238	281	62	262	264	183	284	213	318	302	245
198	267	253	250	225	278	274	265	244	245	

1453.0_1344EC12	417	376	211	339	359	374	403	258	736	220
328	453	385	438	461	535	347	308	408	399	426
407	251	503	357	271	467	404	347	999	353	967
962	955	425	511	596	257	541	387	427	350	312
305	340	635	312	240	368	345	264	367	325	444
359	490	495	502	309	299	491	309	502	317	561
308	589	593	567	300	344	307	595	432	368	287
361	455	339	352	472	394	209	355	410	497	507
518	538	510	316	539	167	640	503	638	497	525
501	646	660	167	649	138	662	275	314	502	495
347	514	512	491	308	413	309	635	269	634	410
414	265	249	518	480	360	314	290	367	377	342
320	360	306	294	316	318	158	275	280	278	168
343	284	366	414	379	356	370	391	366	396	354
360	404	399	525	516	353	521	374	540	499	569
371	167	303	441	495	493	230	334	104	352	356
301	274	320	347	171	189	326	321	366	176	345
447	479	176	251	339	403	725	228	187	482	169
325	472	543	276	358	360	361	458	415	237	351
351	227	404	502	280	472	349	349	416	248	506
325	621	166	225	389	114	273	260	577	285	253
325	0	321	291	367	273	382	356	622	536	26
271	120	336	468	336	508	223	299	563	571	462
353	345	311	326	393	298	373	242	342	313	465
217	506	549	266	360	312	241	406	247	68	496
361	466	556	317	287	333	523	311	496	91	489
7	537	138	555	287	449	550	251	587	305	516
444	533	276	478	317	305	290	336	285	491	350
350	183	353	504	552	596	342	448	554	319	335
176	324	533	462	459	454	266	343	308	364	584
348	315	337	471	454	411	484	367	176	388	365
307	359	83	519	370	124	463	152	481	501	413
260	354	296	337	259	358	281	373	321	274	

253

1456.9_1164EK04	388	370	236	544	458	390	474	291	487	454
304	397	359	474	322	394	442	284	286	405	464
645	245	418	456	299	353	380	638	353	999	367
355	339	305	349	437	224	415	444	493	531	282
286	386	430	521	242	358	468	273	334	380	358
561	441	441	444	557	360	435	313	447	290	331
327	435	340	336	303	340	361	360	289	358	419
267	319	395	257	306	321	240	307	271	402	420
432	410	452	350	454	250	376	427	382	429	393
430	362	359	203	390	227	364	323	459	429	429
308	357	361	410	658	317	310	275	317	269	334
316	358	280	385	389	292	321	327	356	335	317
360	334	310	310	554	349	199	685	368	431	214
336	341	303	347	313	289	322	352	334	349	279
303	340	292	371	376	351	364	331	399	358	393
364	185	230	332	378	381	268	285	82	291	298
290	204	280	295	169	226	348	350	319	159	504
357	269	172	329	387	474	524	279	344	431	145
323	294	348	225	270	347	436	315	639	207	357
309	280	354	416	925	317	434	474	282	262	321
497	385	239	289	432	301	273	331	397	540	244
261	0	296	238	451	437	598	339	343	491	194
363	98	460	341	345	469	239	453	364	448	401
252	250	291	289	281	382	334	258	389	391	414
271	375	452	247	331	271	350	293	221	151	553
207	336	406	242	375	269	430	277	412	190	380
4	275	236	355	437	330	386	294	413	662	471
345	392	350	439	285	285	290	249	358	418	308
352	185	304	391	346	434	382	360	478	310	338
352	242	498	368	369	368	183	288	358	326	378
294	253	386	440	406	308	429	396	156	326	260
329	301	90	313	352	188	379	201	387	400	361
253	293	286	293	243	320	256	301	267	298	

254

1461.7_1135EC00	386	347	64	322	351	348	404	272	687	249
	339	470	370	401	511	511	339	330	463	380
	427	232	514	300	266	420	377	307	967	999
	931	923	433	489	538	59	471	360	439	318
	312	329	624	301	215	397	378	227	393	455
	344	455	457	465	347	297	458	314	484	531
	288	545	589	541	277	329	306	574	463	287
	360	429	308	362	438	366	193	365	401	482
	495	527	479	358	515	137	627	471	628	517
	468	632	663	62	650	118	664	243	284	472
	319	510	511	483	321	391	289	610	285	433
	400	262	255	528	473	353	220	248	364	347
	290	320	283	301	307	202	62	268	293	150
	280	224	356	403	366	341	369	385	361	350
	386	411	377	489	492	357	485	363	502	532
	346	49	251	414	449	460	227	354	125	377
	338	241	319	377	49	190	254	331	337	361
	397	461	92	221	318	404	678	260	205	23
	281	442	556	266	359	352	316	423	419	321
	337	96	356	485	288	523	317	325	463	515
	316	574	224	226	408	1	288	263	602	248
	423	0	350	289	336	270	344	330	586	0
	226	148	348	453	334	496	168	299	578	423
	300	389	275	281	389	266	339	68	368	488
	188	503	559	340	365	296	180	379	139	454
	343	456	567	263	275	327	505	259	474	477
	1	534	129	526	241	414	546	264	571	497
	417	526	249	480	296	235	142	243	277	349
	338	185	328	474	530	597	351	445	588	284
	197	234	508	452	437	444	276	340	329	628
	320	364	334	501	473	413	439	371	192	360
	311	350	62	484	359	43	415	109	438	398
	238	338	232	266	207	321	167	307	204	236

1464.3_1344EC12	417	377	234	321	338	371	399	249	721	237
322	467	409	446	492	495	334	327	418	400	425
422	262	490	359	285	476	416	334	962	355	931
999	979	433	498	577	261	525	383	422	347	316
303	354	641	305	241	378	332	259	355	334	450
349	485	489	496	320	297	487	305	487	313	576
304	575	608	584	314	347	314	605	420	345	300
329	455	349	360	462	405	215	350	405	505	495
506	524	496	341	541	168	654	516	652	487	514
489	660	668	196	656	142	666	279	315	496	487
348	501	498	479	320	423	320	652	261	653	420
425	286	232	496	469	364	301	304	361	389	353
306	381	294	282	322	302	186	302	290	282	172
331	292	372	386	376	360	361	376	345	392	339
360	386	392	534	517	350	521	341	533	509	560
370	178	279	436	518	510	224	328	104	349	350
309	266	316	339	182	189	314	313	363	174	336
438	482	159	260	333	399	725	232	199	482	181
342	425	531	278	351	374	340	452	439	242	357
374	260	404	521	257	488	348	329	427	193	500
303	617	161	236	377	97	260	290	560	284	244
359	0	343	308	361	281	369	360	617	528	25
260	122	342	471	311	508	226	293	567	551	462
404	348	313	312	413	312	366	214	340	317	478
230	513	539	298	368	315	257	395	242	101	516
368	463	545	292	286	342	502	297	485	80	476
7	566	148	565	294	402	534	237	559	323	495
443	547	285	477	330	299	297	317	310	497	348
346	184	360	498	538	595	329	439	536	314	328
199	303	532	464	454	447	254	349	300	361	603
371	328	329	470	470	389	482	364	180	392	351
317	358	94	559	371	127	469	203	503	524	412
279	334	290	317	250	371	261	357	300	259	

1467.9_1135EC00	410	364	161	322	351	384	391	268	707	224
319	464	404	424	493	512	331	316	492	419	409
398	238	490	329	292	473	435	343	955	339	923
979	999	429	491	557	193	497	379	415	327	312
303	355	645	305	248	362	331	242	376	314	450
343	470	466	471	312	312	467	305	485	322	565
311	563	596	574	315	337	334	594	461	342	288
351	459	317	376	472	398	185	361	395	492	484
498	515	485	338	535	155	662	531	663	466	502
472	668	682	134	665	127	681	262	300	487	480
327	505	503	481	318	407	295	648	265	650	428
408	267	230	494	470	354	269	271	364	365	352
289	354	294	277	303	262	132	287	289	285	157
304	259	379	387	384	364	371	384	350	387	337
358	379	380	519	503	345	498	332	506	481	535
361	137	269	412	498	488	219	320	106	337	338
321	252	309	329	144	187	283	320	333	156	335
429	473	172	236	352	391	699	238	177	492	89
333	447	508	272	356	384	317	438	414	245	321
379	202	396	527	254	549	328	324	416	204	488
279	607	155	218	377	105	255	308	555	284	254
423	0	352	287	337	262	346	335	619	517	21
209	126	359	466	272	522	191	287	600	548	469
371	347	328	321	397	279	365	97	334	292	467
208	498	543	306	377	311	176	384	203	95	465
377	459	560	295	245	336	491	314	472	96	462
7	565	137	561	264	395	539	236	546	306	496
429	553	253	493	329	269	232	298	276	516	351
352	189	368	495	546	616	329	432	553	291	289
199	290	526	456	459	447	244	370	304	375	596
357	331	318	464	451	399	456	345	176	375	340
291	341	86	537	351	80	451	192	479	499	401
257	318	265	302	201	330	259	321	222	272	

1475.1_1288EC45	329	301	158	278	264	275	253	246	499	181
244	287	333	334	575	578	273	362	530	401	351
352	338	395	269	262	462	375	267	425	305	433
433	429	999	498	499	200	434	281	335	277	331
324	299	441	292	195	424	398	206	264	236	430
282	368	383	386	311	339	380	285	431	252	360
268	444	384	370	242	345	230	366	413	341	327
319	339	275	466	339	458	195	339	369	443	396
389	381	405	324	410	167	410	432	405	488	391
489	407	387	245	403	152	398	198	278	507	516
310	384	391	406	298	326	291	427	270	424	376
310	239	175	415	384	327	219	222	314	428	404
305	263	263	238	278	149	232	271	286	276	244
257	166	359	370	392	349	351	404	343	422	330
327	330	325	421	408	319	415	333	408	409	435
338	223	267	391	397	374	222	314	172	303	305
262	243	292	267	239	153	308	271	365	245	259
415	436	187	192	271	253	482	202	163	316	114
307	539	447	300	496	339	351	485	371	359	264
303	178	258	351	204	443	293	238	947	230	521
219	556	203	310	358	0	315	222	417	311	185
476	0	502	226	305	340	290	279	418	390	24
217	115	334	503	263	455	132	365	422	459	434
279	405	312	277	421	205	330	82	394	310	474
130	446	374	399	353	301	188	442	186	204	491
281	409	485	268	198	311	416	342	367	213	413
246	408	130	374	251	455	389	235	406	308	456
361	435	205	377	289	254	194	281	264	391	416
339	164	325	421	394	431	229	350	382	272	268
266	267	400	404	370	373	273	322	344	340	429
314	285	445	332	308	354	436	401	241	425	328
362	333	189	347	404	168	361	212	404	364	357
269	324	278	320	304	332	233	350	266	278	

258

1488.5_1288EC44	358	287	214	316	333	319	321	287	551	251
376	301	354	407	594	513	303	507	484	401	410
402	279	454	326	252	471	378	295	511	349	489
498	491	498	999	568	236	487	356	463	298	395
311	297	497	317	164	437	420	293	304	270	544
340	510	528	531	361	320	531	305	483	306	381
284	520	425	388	296	373	252	403	450	350	289
391	424	311	433	437	470	232	364	466	466	478
512	464	502	364	490	225	477	486	475	545	457
546	475	441	156	450	185	446	210	273	550	549
378	483	489	501	337	386	252	515	338	518	442
430	237	237	495	449	459	240	238	402	385	487
387	289	276	288	300	152	156	354	296	230	189
271	180	329	391	341	331	338	362	345	467	349
425	390	407	434	422	387	425	424	485	410	486
418	157	239	427	403	400	170	405	321	474	418
420	396	455	440	194	234	313	462	374	139	325
517	529	123	225	299	321	556	284	228	355	172
346	493	504	299	582	419	318	570	438	358	255
390	179	309	365	226	545	273	248	536	291	967
202	607	108	254	433	107	329	209	441	333	185
494	0	402	314	291	286	335	253	460	552	46
210	100	345	475	324	549	156	339	540	521	471
216	404	381	239	343	227	350	151	463	355	491
155	428	486	435	440	395	221	469	254	86	533
328	491	441	266	201	345	551	345	505	210	334
285	456	104	493	221	536	473	264	503	303	484
440	535	207	433	355	222	163	276	254	446	525
351	203	313	494	457	435	233	501	478	248	223
262	267	456	472	387	418	271	320	403	320	476
330	410	407	395	371	387	414	461	330	408	389
423	363	165	380	475	200	350	147	414	399	407
285	339	240	288	260	319	216	339	279	240	



259

1494.1_1135EC00	344	301	40	326	315	328	352	280	730	221
276	360	318	354	483	450	280	367	356	394	454
454	274	530	290	250	435	328	358	596	437	538
577	557	499	568	999	44	821	403	400	306	332
336	326	648	368	183	397	332	267	318	299	552
357	742	748	751	295	386	744	355	827	297	516
348	878	534	524	288	385	275	544	363	408	284
446	544	253	444	411	485	248	384	519	738	832
825	759	822	311	805	154	678	714	707	838	751
838	681	711	82	725	162	713	258	274	787	787
361	705	713	788	377	486	256	556	376	563	518
492	232	336	634	614	470	292	243	385	388	628
372	352	295	368	298	166	76	364	281	248	139
309	172	458	545	469	442	464	495	438	508	449
502	624	458	679	695	462	669	596	780	647	781
492	35	291	674	635	650	224	443	211	456	454
399	419	448	485	78	291	342	493	549	47	355
410	427	163	175	304	352	738	243	141	383	100
288	432	561	249	359	344	431	448	443	281	277
301	167	262	373	343	438	264	288	389	225	566
250	904	84	247	341	139	310	298	587	373	245
415	0	454	247	334	258	371	256	745	808	36
206	178	434	470	285	748	195	432	661	847	613
328	408	304	236	478	224	404	86	636	276	655
144	628	671	493	633	353	222	426	182	46	667
307	752	594	305	212	333	822	464	784	118	596
443	555	111	610	244	482	761	242	772	367	723
714	678	206	613	342	255	180	298	263	586	640
448	239	344	588	641	747	451	529	733	289	254
185	278	708	562	671	619	286	444	629	473	621
470	402	599	639	632	518	456	661	307	543	472
585	488	204	522	629	139	602	101	650	648	658
310	502	272	283	265	322	254	347	265	266	

1500.0_1135EC03	205	182	842	239	230	158	220	174	159	217
346	121	171	198	221	216	162	274	259	227	142
188	261	35	147	282	171	201	147	257	224	59
261	193	200	236	44	999	371	134	262	177	311
304	225	0	212	172	254	231	202	244	215	142
199	261	261	250	200	106	275	214	6	209	245
225	120	244	237	195	246	258	242	301	252	195
257	283	221	210	200	289	220	216	247	248	181
216	157	173	2	180	318	254	193	245	178	166
229	265	227	801	313	232	267	285	172	245	226
0	165	78	103	263	281	107	219	169	225	323
290	136	218	176	165	3	113	166	172	227	231
170	189	297	212	199	218	814	127	371	1	253
193	200	267	216	291	290	274	290	237	269	282
290	164	256	205	197	251	205	205	196	237	229
244	764	153	223	187	194	295	53	0	0	141
4	0	128	0	674	65	275	0	213	712	191
127	177	280	148	174	220	6	93	202	44	320
132	0	214	252	238	206	0	0	144	0	168
151	126	148	166	144	228	249	129	171	6	77
20	0	183	42	118	1	271	99	56	175	237
178	0	90	201	202	171	163	84	0	236	65
172	169	146	0	44	2	130	230	0	8	212
127	24	118	397	0	226	23	43	141	202	0
204	203	2	0	86	0	185	79	197	175	234
223	0	245	156	209	135	38	6	62	91	96
0	226	0	0	174	7	6	230	9	113	236
0	192	166	120	181	311	223	257	242	116	7
58	0	1	283	218	2	122	5	233	286	277
0	257	230	168	0	249	67	6	120	176	0
60	151	245	101	311	1	266	13	0	266	201
0	150	0	73	221	0	0	177	77	0	4
210	3	193	287	123	167	214	173	151	145	

1502.4_1288EC34	361	297	260	347	315	301	347	260	624	262
366	351	300	360	438	426	280	396	445	407	427
419	297	467	289	331	433	324	337	541	415	471
525	497	434	487	821	371	999	367	393	295	380
400	341	586	333	195	441	372	245	341	323	519
335	672	682	676	309	379	678	378	713	303	488
349	750	485	492	288	398	315	487	405	387	344
391	504	333	412	381	496	240	382	497	629	730
727	655	719	292	712	201	617	643	640	740	632
743	622	637	351	673	196	646	313	337	715	711
334	619	622	690	349	458	244	550	354	547	567
487	245	328	590	574	444	280	211	379	421	586
346	319	364	357	346	223	313	294	354	266	219
309	256	431	513	458	439	440	500	442	477	440
489	553	410	600	607	474	575	518	673	573	685
471	302	266	589	537	545	269	397	189	410	420
387	394	409	418	333	300	357	474	504	318	332
390	409	241	180	283	347	651	197	171	340	212
254	379	574	277	345	335	409	392	416	258	287
293	127	272	384	320	439	359	325	315	219	481
252	799	87	241	312	44	344	253	556	325	256
425	0	427	298	399	299	333	327	639	715	195
240	235	428	383	270	689	207	444	576	749	580
325	353	264	359	456	272	354	119	608	323	616
127	611	635	411	591	266	271	366	198	123	630
364	666	541	278	270	267	743	444	700	140	532
429	496	141	561	285	401	677	240	679	335	673
646	671	262	565	281	318	199	308	266	538	603
430	117	288	605	587	663	389	516	641	332	297
203	305	655	528	613	597	283	400	586	428	560
439	356	620	606	644	472	472	601	265	559	471
523	483	190	468	552	137	528	154	574	571	595
367	461	298	340	280	333	238	335	248	284	

1510.5_1164EK04	511	386	141	474	443	578	455	216	373	381
337	377	465	412	329	329	413	290	253	401	364
429	309	368	603	259	445	425	395	387	444	360
383	379	281	356	403	134	367	999	367	323	288
309	415	333	345	221	386	372	271	419	445	327
343	382	393	388	316	500	385	301	356	273	367
297	365	385	367	278	303	425	371	284	265	402
276	287	441	288	267	353	226	367	290	416	360
387	421	373	303	407	210	356	386	354	384	421
388	342	333	140	334	145	337	395	407	398	397
235	282	284	308	373	309	334	320	246	315	294
295	293	215	334	312	259	244	366	335	450	317
264	338	329	233	341	451	130	308	294	309	234
264	549	286	348	283	294	278	320	298	360	310
273	315	334	367	367	314	352	290	341	368	358
323	96	307	321	355	348	222	251	86	230	256
172	61	219	240	89	212	288	265	306	102	455
422	352	208	376	544	455	399	210	318	384	197
387	282	314	208	279	324	240	375	431	276	480
436	325	414	441	374	269	374	506	272	61	345
292	409	248	283	343	153	284	512	339	362	210
308	0	320	350	437	330	323	310	358	407	27
296	110	550	319	355	383	263	380	330	396	427
256	275	209	422	241	480	306	275	347	387	357
291	401	372	256	261	275	389	263	225	140	477
166	301	363	292	444	14	394	245	393	154	353
2	305	109	297	398	279	311	126	334	342	441
314	342	470	367	266	286	275	330	424	322	285
305	36	380	322	311	454	429	365	511	310	314
234	322	534	299	334	320	184	239	340	256	442
256	220	376	420	419	351	404	367	203	343	289
316	304	163	325	324	172	337	66	358	330	302
257	273	309	300	265	330	196	328	326	233	

263

1519.2_1185EK09	353	304	270	375	333	323	379	204	445	307
253	385	421	585	329	396	339	250	338	514	472
482	209	433	420	290	383	486	476	427	493	439
422	415	335	463	400	262	393	367	999	407	240
213	368	421	429	204	326	320	308	280	302	368
437	334	348	360	377	464	345	259	358	218	390
231	352	408	387	240	256	337	391	295	283	307
288	378	349	237	312	342	187	259	276	333	265
275	306	310	466	300	187	377	403	362	357	303
358	351	316	199	326	176	335	317	343	387	362
232	320	334	361	498	325	340	290	289	290	301
267	262	176	306	327	244	251	331	261	413	271
289	381	300	214	371	352	194	464	351	353	152
276	342	273	250	275	284	259	269	259	319	267
246	255	245	373	364	232	352	285	339	341	345
263	206	229	339	349	353	179	241	36	239	252
154	58	190	248	196	204	283	221	279	200	385
396	369	68	388	331	379	481	225	286	407	199
376	389	382	261	306	473	388	442	479	314	348
373	281	372	454	429	337	395	425	401	117	464
291	374	289	347	986	124	176	239	337	457	147
284	0	280	269	430	301	485	324	409	373	150
245	57	506	437	375	367	206	392	381	390	376
269	307	280	261	371	360	335	238	369	303	339
226	399	301	266	316	341	324	341	231	171	491
278	379	341	245	298	235	314	327	311	122	290
12	323	214	345	325	351	359	138	350	538	367
348	354	348	391	307	299	333	281	395	372	275
313	179	356	363	327	383	332	356	403	264	316
299	276	372	290	337	261	221	254	280	214	385
318	270	328	313	316	311	400	332	152	350	227
287	249	120	338	315	210	343	211	378	364	328
214	255	229	273	244	311	238	276	251	229	

264

1523.1_1164EK04	347	393	187	391	347	323	345	234	317	262
298	345	371	349	302	321	336	234	309	409	326
480	206	332	348	275	318	416	372	350	531	319
347	327	277	298	306	177	295	323	407	999	270
276	362	381	306	244	343	397	261	305	374	314
395	266	268	263	516	326	252	282	297	232	304
270	286	313	303	277	252	376	308	277	248	352
265	298	393	254	322	324	260	276	249	293	255
259	275	266	353	299	255	324	303	315	285	271
290	305	290	235	290	220	303	329	412	302	302
279	255	258	276	366	305	303	245	332	236	266
275	347	288	273	293	290	302	338	248	346	246
319	351	290	307	607	346	230	553	363	392	179
319	348	276	272	305	327	280	313	319	329	286
282	260	298	303	301	285	306	246	296	312	298
277	195	208	230	293	303	249	231	98	231	237
184	129	215	248	184	219	312	277	215	155	371
362	318	149	319	323	345	350	234	242	369	157
368	272	289	221	255	337	277	278	489	190	287
370	219	382	443	486	291	425	366	274	276	274
560	283	253	283	383	781	254	250	333	316	238
224	228	242	207	343	375	401	321	268	307	8
301	73	356	264	317	285	211	392	259	314	314
203	260	244	248	205	347	272	180	253	333	275
234	260	321	211	239	273	323	288	205	163	350
202	279	297	206	383	197	260	280	246	171	305
2	261	245	304	422	287	293	186	290	382	341
293	301	366	331	232	282	290	238	358	333	221
312	154	352	284	267	329	295	313	344	272	277
325	228	349	272	280	263	262	274	225	253	276
278	256	263	333	307	307	346	274	159	248	241
235	260	122	294	242	216	298	198	299	326	284
248	224	307	271	259	295	283	288	281	243	

265

1526.0_1185EK10	267	241	252	196	213	252	316	256	403	286
	305	260	283	401	339	377	295	271	347	321
	333	260	308	268	366	375	298	228	312	282
	316	312	331	395	332	311	380	288	240	270
	408	331	335	197	195	327	432	204	196	268
	210	318	321	318	226	367	310	266	346	254
	282	304	316	272	280	292	272	282	341	384
	309	267	322	302	271	368	179	222	293	306
	278	291	300	290	291	227	342	344	342	384
	380	324	311	305	299	269	316	197	418	386
	182	310	313	333	181	250	168	289	278	283
	258	236	200	353	353	321	205	147	137	358
	255	254	241	218	218	269	279	261	190	150
	236	296	275	285	264	283	261	293	265	352
	311	313	388	318	314	339	300	267	296	295
	368	264	244	312	308	293	203	278	160	153
	119	29	192	257	249	196	330	245	294	254
	329	304	137	262	237	316	403	306	272	279
	263	382	313	283	340	366	192	349	349	293
	258	271	269	316	234	281	341	304	363	211
	136	367	157	343	318	37	405	401	320	224
	322	0	373	305	348	395	240	326	348	333
	277	51	403	409	181	373	282	290	342	348
	286	352	273	289	397	295	391	247	282	346
	143	384	380	184	271	348	295	353	225	193
	214	323	285	242	310	120	283	280	308	211
	0	301	179	304	373	336	325	191	330	266
	296	332	303	328	323	277	302	292	262	337
	316	114	238	399	334	339	232	361	327	271
	221	266	274	284	319	282	258	277	306	248
	268	306	356	301	336	276	380	324	315	335
	266	295	164	252	322	247	262	200	327	297
	386	288	257	327	274	315	228	303	270	271

266

1530.9_1185EK13	271	256	278	298	274	248	269	249	374	266
279	245	293	393	330	327	307	272	396	264	263
285	211	372	263	327	300	310	258	305	286	312
303	303	324	311	336	304	400	309	213	276	408
999	306	385	246	214	460	474	194	224	265	285
252	231	241	222	241	276	219	243	297	197	248
246	313	262	253	246	210	253	256	295	265	621
250	221	287	256	251	305	197	266	298	313	263
292	323	288	240	306	193	333	276	342	240	319
253	316	301	254	245	203	270	204	549	250	252
265	278	280	281	255	225	227	268	227	263	315
195	255	179	279	288	257	156	177	193	260	240
236	206	252	231	243	271	224	248	230	169	232
211	348	235	221	266	261	243	285	286	329	254
238	233	266	258	238	249	254	217	269	257	286
272	211	217	208	262	231	202	171	160	152	181
198	220	185	167	230	182	249	232	213	214	301
316	250	147	242	264	269	389	261	273	277	244
308	300	291	272	326	305	199	315	312	191	288
264	280	259	308	244	302	343	238	342	237	314
135	359	228	358	285	74	974	354	353	182	195
292	0	354	240	297	458	244	272	324	279	123
287	93	301	271	204	290	350	308	336	323	286
202	372	229	264	311	279	292	195	278	605	270
151	361	271	263	236	296	266	302	245	258	365
206	331	311	214	402	187	328	277	268	125	250
0	231	154	304	514	390	322	235	318	236	296
280	324	286	305	254	253	328	248	213	284	220
252	73	262	327	257	305	240	352	312	255	295
191	243	277	282	247	246	178	271	205	276	346
305	229	264	422	440	268	326	251	212	303	273
274	249	109	274	226	227	257	109	269	294	234
254	223	273	290	263	277	207	254	197	256	



267

1533.6_1344EC21	348	346	243	384	378	336	375	207	342	350
368	383	679	435	319	361	359	292	349	410	367
417	261	368	566	301	310	608	388	340	386	329
354	355	299	297	326	225	341	415	368	362	331
306	999	335	280	166	351	445	256	382	660	358
336	329	311	320	347	319	316	357	292	308	334
340	319	328	338	327	295	667	305	229	262	328
252	276	608	284	278	357	184	357	319	352	320
315	329	326	350	333	213	322	307	315	315	339
321	316	274	187	302	192	301	658	548	345	344
253	295	292	297	343	310	218	360	267	364	331
293	313	180	312	293	294	211	677	293	407	303
289	318	321	251	326	473	184	292	273	249	201
251	490	281	306	305	304	269	306	318	352	294
276	300	311	324	311	289	316	266	306	311	314
308	173	177	289	321	308	201	258	102	254	277
260	250	264	251	173	263	320	280	281	172	379
375	310	50	701	297	375	357	203	242	390	236
635	334	276	244	326	363	252	364	401	259	323
323	485	345	372	314	310	445	470	349	220	309
283	355	185	265	373	222	314	462	344	317	173
308	0	299	349	383	436	356	431	369	342	175
229	137	331	269	365	342	269	361	363	331	340
219	312	386	300	288	616	334	425	338	349	342
525	319	331	299	286	283	527	332	214	149	376
209	318	320	176	606	252	345	243	312	82	367
0	292	140	255	547	261	279	196	323	354	357
291	374	664	307	292	239	466	220	672	298	348
282	37	662	337	308	448	491	574	450	237	271
159	203	458	306	325	321	268	263	299	269	346
259	297	319	347	347	329	349	293	238	311	277
311	322	145	298	287	167	328	114	331	286	319
290	276	256	274	237	301	193	273	254	230	

268

1559.6_2011EC33	365	387	0	388	407	304	346	220	646	204
366	445	382	425	505	525	324	386	481	409	343
505	262	505	311	299	444	453	376	635	430	624
641	645	441	497	648	0	586	333	421	381	335
385	335	999	458	213	418	376	259	410	335	682
376	538	535	541	365	288	529	289	590	282	440
257	617	468	453	245	361	360	453	417	351	347
304	421	350	400	451	431	215	386	422	510	537
546	490	551	367	544	129	549	546	525	674	504
676	533	545	164	539	150	554	301	377	637	642
337	571	558	568	402	429	281	513	338	518	613
492	249	234	726	672	534	260	298	368	342	436
309	380	264	318	353	181	137	337	283	314	156
321	234	318	374	352	313	324	399	397	421	397
325	433	418	507	509	392	497	410	564	501	569
408	0	264	528	473	490	229	379	110	389	387
341	337	357	376	0	250	242	443	429	0	385
444	450	9	268	312	346	648	226	177	496	29
343	428	714	247	461	353	315	443	478	549	294
347	14	353	425	323	530	357	314	448	300	511
325	658	171	281	363	8	391	306	889	473	199
445	0	399	287	325	284	386	381	593	538	0
248	72	328	535	236	593	155	383	551	647	474
346	424	385	279	386	255	326	74	489	340	759
159	467	552	464	447	284	205	403	101	125	526
292	548	505	285	274	331	550	334	545	38	575
15	512	23	513	304	433	606	269	604	403	572
471	712	272	558	325	249	141	266	309	556	489
355	205	422	545	542	618	302	508	541	314	224
227	249	503	494	509	442	321	335	464	371	582
381	303	439	450	440	387	416	452	334	524	387
423	380	213	391	456	77	455	234	476	474	455
249	409	245	259	270	249	233	287	193	260	

269

1560.6_1164EK04	275	261	258	409	332	299	331	166	403	306
224	307	279	363	268	346	324	241	317	342	537
507	216	351	378	260	278	309	569	312	521	301
305	305	292	317	368	212	333	345	429	306	197
246	280	458	999	128	286	287	289	243	271	276
560	300	312	296	336	393	294	234	347	223	269
237	340	240	269	205	248	246	258	279	251	291
277	328	251	250	267	293	248	215	276	287	298
310	291	325	307	302	225	338	353	325	353	287
358	307	320	187	315	185	324	265	308	362	365
235	305	306	331	680	229	183	275	263	272	274
211	196	166	288	288	229	224	253	256	312	259
269	298	268	264	289	256	183	479	264	305	161
289	304	248	276	247	233	251	282	282	301	244
248	277	223	338	341	275	324	269	358	347	340
277	181	173	313	318	338	180	255	71	255	258
248	139	258	242	173	182	263	289	252	191	367
347	332	55	183	346	331	402	168	257	341	115
325	309	340	188	271	322	414	302	509	219	227
321	159	288	286	443	281	306	350	332	169	324
192	329	233	190	388	70	188	222	366	900	146
240	0	256	221	300	271	546	268	345	332	133
151	48	417	271	244	359	193	350	319	360	382
295	252	235	214	221	252	247	228	366	286	266
142	266	298	261	285	305	251	284	208	78	415
139	334	271	187	246	314	300	245	337	106	366
8	271	69	282	256	323	309	351	321	670	373
309	309	238	508	257	199	219	220	275	504	237
312	225	152	300	310	340	176	278	355	239	245
256	220	315	294	284	280	236	261	281	232	272
294	238	277	295	265	297	303	285	136	295	237
267	250	109	313	268	104	316	156	303	310	300
163	214	211	238	215	272	178	235	192	210	

270

1565.2_1164EK04	232	359	30	235	213	258	187	170	216	91
212	306	166	202	214	257	146	186	240	227	141
210	248	228	174	220	219	185	234	240	242	215
241	248	195	164	183	172	195	221	204	244	195
214	166	213	128	999	207	230	254	261	194	200
320	223	190	205	261	195	192	168	184	192	189
173	199	227	197	171	179	176	206	230	190	228
194	270	212	176	230	203	222	198	273	236	204
219	219	192	142	220	131	196	218	197	186	211
187	199	210	135	206	110	237	217	195	219	215
213	179	178	180	249	174	306	220	226	221	187
182	220	200	213	191	161	236	187	205	178	161
258	287	200	175	209	197	173	195	223	183	111
219	175	185	196	174	191	182	221	200	227	219
215	192	231	197	190	180	203	178	210	216	204
200	118	110	185	211	208	182	246	7	242	248
57	11	188	221	20	116	252	211	195	30	245
165	170	180	122	224	187	198	187	49	315	3
99	201	219	82	144	140	207	139	196	77	323
143	197	265	285	226	182	180	186	109	0	120
250	174	49	138	178	164	182	225	223	99	929
172	0	236	163	216	167	290	174	216	200	0
227	160	206	145	119	189	110	157	222	209	235
60	112	139	156	145	207	126	0	155	172	209
194	201	256	5	131	127	166	146	146	0	193
146	98	248	134	208	82	222	172	212	51	178
317	153	182	168	161	218	194	56	208	231	240
207	220	170	248	150	181	195	150	180	177	110
60	2	159	189	193	227	212	227	237	181	134
91	142	200	208	234	198	162	126	116	192	185
129	155	199	209	207	168	214	169	8	114	211
174	203	19	223	172	59	180	88	229	203	219
152	135	221	192	176	239	188	219	241	166	

271

1608.3_2011EC27	302	315	213	311	276	331	299	311	435	287
254	246	377	388	418	477	267	359	374	319	370
365	220	402	348	325	458	348	326	368	358	397
378	362	424	437	397	254	441	386	326	343	327
460	351	418	286	207	999	428	327	306	322	387
303	297	316	309	320	281	295	346	319	369	281
341	366	350	285	368	338	273	326	459	358	430
340	332	313	367	378	440	285	351	289	388	275
301	390	342	364	354	234	347	417	346	358	386
379	333	325	263	342	222	350	232	433	373	377
320	307	308	322	300	252	319	324	302	322	376
267	353	171	335	337	305	303	257	359	391	312
359	340	276	175	321	369	218	321	371	320	208
329	361	342	326	328	329	325	344	336	396	338
314	290	353	348	341	302	346	322	330	360	360
350	214	228	350	339	330	219	236	181	233	233
304	232	250	186	299	221	392	280	317	236	304
380	456	211	280	313	299	428	298	282	288	141
351	466	377	370	451	345	373	388	399	283	285
316	307	343	372	250	368	348	320	488	219	442
208	397	213	339	366	110	429	333	403	306	236
380	136	434	347	370	391	340	389	390	344	371
361	191	327	426	440	408	363	383	389	354	393
397	469	338	344	315	343	372	342	349	453	358
185	457	285	311	318	322	274	345	393	239	504
359	378	379	229	344	255	357	269	335	261	339
232	281	251	320	411	464	343	319	354	358	370
371	368	298	369	338	344	365	262	264	403	346
346	241	330	381	312	381	231	380	411	367	339
333	261	404	353	356	350	315	318	283	330	413
347	321	346	476	461	298	445	357	306	445	379
330	309	231	314	365	189	386	242	361	366	339
322	345	455	492	396	457	335	453	420	294	

272

1627.1_1185EK12	324	293	237	389	325	319	370	266	389	359
259	329	393	420	344	418	369	364	304	386	422
404	210	340	408	308	374	391	356	345	468	378
332	331	398	420	332	231	372	372	320	397	432
474	445	376	287	230	428	999	213	264	339	343
350	283	284	284	392	313	277	280	301	237	247
289	277	275	255	256	273	323	275	274	325	419
257	315	356	325	296	332	204	326	268	335	251
268	289	283	329	284	220	339	374	345	350	282
354	340	332	237	334	199	331	276	505	368	364
276	269	270	289	334	250	303	248	262	243	316
252	275	263	297	295	276	282	240	237	342	264
274	308	280	271	474	363	209	457	328	226	186
292	359	287	281	309	304	271	319	323	359	276
343	265	342	354	347	351	337	238	345	350	328
350	187	232	317	349	333	184	253	129	262	267
280	278	217	268	206	229	321	288	295	161	360
366	282	126	323	327	370	440	242	328	325	162
352	443	356	254	434	338	410	360	436	223	342
316	296	314	372	418	333	449	393	454	195	424
390	348	240	368	368	208	478	437	379	323	174
266	0	359	295	358	927	376	320	351	293	44
297	92	362	440	271	369	275	395	397	330	371
340	399	269	309	270	343	352	270	288	476	255
242	346	380	241	281	279	306	373	248	207	491
254	355	379	254	424	307	291	257	279	189	348
9	310	182	322	493	389	296	235	308	359	388
340	309	337	329	240	281	349	246	321	396	265
330	137	301	343	268	360	280	406	327	320	304
248	238	423	386	337	305	285	319	249	305	397
365	319	296	403	430	267	423	299	253	313	328
267	271	116	321	304	185	383	213	349	352	336
254	270	304	343	325	331	265	320	301	280	

273

1628.2_1344EC22	298	308	189	246	235	255	252	232	255	160
	208	244	250	298	239	215	205	216	226	249
	297	214	306	276	194	269	288	268	264	227
	259	242	206	293	267	202	245	271	308	204
	194	256	259	289	254	327	213	999	239	254
	348	225	206	218	266	251	204	304	210	230
	302	218	263	225	228	312	254	233	210	245
	225	221	255	218	277	324	609	197	275	243
	248	226	218	174	237	261	206	257	202	225
	257	193	190	174	197	306	215	251	282	299
	252	199	197	211	287	200	223	231	284	159
	208	235	224	197	174	212	289	233	358	253
	265	335	269	258	206	249	175	238	249	176
	300	247	222	278	249	266	251	303	295	246
	215	208	180	222	215	281	213	194	248	248
	302	176	234	239	217	215	276	195	78	218
	184	128	233	211	156	114	347	262	226	220
	262	322	239	197	243	252	272	218	123	147
	232	101	282	154	223	186	204	317	307	284
	203	243	252	306	246	223	236	302	200	292
	183	290	103	166	301	167	176	230	255	255
	290	215	252	137	266	193	337	226	231	136
	253	123	265	252	241	268	213	249	242	336
	238	125	194	203	227	296	211	174	193	168
	192	305	193	199	236	194	221	197	306	331
	163	209	250	259	253	139	225	196	220	244
	159	197	253	214	264	268	212	184	213	241
	213	228	265	240	185	300	215	270	302	231
	255	69	190	249	198	226	223	218	223	265
	189	267	265	307	240	204	212	199	215	179
	160	169	199	272	259	267	337	253	201	200
	184	251	105	230	243	154	214	221	232	219
	184	156	320	290	276	351	327	310	308	227

274

1630.2_1135EC00	330	287	190	328	318	349	255	207	383	200
193	424	352	333	238	293	223	219	304	391	246
362	244	413	367	267	362	364	298	367	334	393
355	376	264	304	318	244	341	419	280	305	196
224	382	410	243	261	306	264	239	999	333	345
278	350	353	349	257	288	348	289	301	281	322
269	263	355	320	274	285	346	317	236	287	298
285	278	323	268	254	321	237	202	256	310	284
296	308	346	290	319	139	276	297	283	255	298
277	264	256	241	276	189	279	337	326	296	303
270	264	262	282	267	303	305	260	296	267	244
245	255	196	264	255	283	262	353	233	351	262
287	338	256	240	327	377	188	288	301	290	212
285	403	213	259	209	226	218	254	267	338	214
246	280	261	300	299	226	306	251	277	293	318
258	186	287	264	317	292	196	207	206	182	217
267	265	186	219	232	223	337	170	269	199	376
283	235	159	319	321	255	394	240	195	449	146
301	241	330	263	276	409	231	379	392	218	409
407	311	402	481	288	366	347	323	285	38	319
274	316	233	228	325	203	250	348	325	257	238
333	237	296	184	356	286	336	284	321	328	178
332	94	301	320	265	371	260	397	383	330	338
208	282	308	314	249	355	349	290	279	302	258
233	286	322	257	228	272	303	253	301	217	380
265	264	316	264	335	233	310	196	371	231	291
2	272	209	278	320	305	243	265	266	343	337
219	261	359	252	304	335	293	288	305	316	215
327	158	338	387	285	341	274	346	379	344	350
207	292	325	271	243	235	286	258	231	227	349
270	221	327	297	328	257	438	279	218	315	298
255	266	190	271	296	177	283	260	305	328	269
257	304	349	373	345	343	269	331	327	322	



275

1636.7_1135ec00	333	313	210	338	328	345	348	174	327	245
290	278	695	365	240	336	319	221	260	361	370
381	210	316	587	295	358	594	401	325	380	296
334	314	236	270	299	215	323	445	302	374	268
265	660	335	271	194	322	339	271	333	999	261
342	263	270	268	372	285	262	328	284	251	264
332	297	263	273	291	262	788	271	225	257	348
231	292	566	264	246	308	189	354	255	292	230
234	255	253	329	262	238	318	346	311	298	250
298	291	268	195	292	170	283	712	633	313	300
237	254	254	258	323	275	240	276	245	276	252
232	266	157	271	276	262	247	766	274	392	280
289	306	262	190	302	580	180	286	325	313	217
273	545	242	258	282	280	272	294	321	318	282
250	279	256	290	282	262	277	233	269	281	269
284	162	218	272	287	283	234	196	135	234	234
237	176	229	245	180	193	245	254	226	174	308
359	317	87	774	334	348	344	164	193	321	103
732	326	257	243	270	315	253	341	399	227	351
334	594	328	377	312	314	444	413	234	139	285
270	326	214	223	346	213	261	522	306	310	199
215	0	249	236	344	355	303	445	302	294	155
255	102	339	242	345	305	311	362	307	316	328
223	275	332	308	227	642	288	492	287	352	275
613	282	289	244	296	271	500	283	232	160	342
200	304	292	231	715	152	283	232	258	29	343
1	227	141	284	635	248	284	222	297	308	323
311	324	729	328	220	242	410	259	721	320	310
313	31	810	309	264	412	591	551	463	240	288
251	246	416	208	330	247	183	214	274	242	319
231	263	283	314	316	287	382	266	199	292	236
288	267	115	251	248	195	324	84	310	328	303
233	210	253	269	236	303	232	269	258	222	

276

1639.3_1135EC00	343	356	123	330	337	297	317	262	478	226
299	424	317	402	505	435	292	318	452	429	356
441	267	446	297	261	397	359	306	444	358	455
450	450	430	544	552	142	519	327	368	314	332
285	358	682	276	200	387	343	254	345	261	999
310	469	453	460	328	335	456	300	491	245	417
252	517	426	425	244	348	270	414	362	313	277
342	391	302	360	476	423	197	347	389	463	477
480	447	492	336	477	218	455	446	461	614	450
616	453	436	183	462	179	444	252	308	617	620
366	457	453	478	303	492	227	409	401	411	588
576	247	309	685	634	654	277	256	334	404	471
369	325	260	387	330	165	175	343	293	246	195
332	191	331	346	362	337	317	384	362	418	397
349	443	315	497	493	399	464	485	489	457	490
417	153	215	469	450	450	189	447	228	435	456
401	357	412	442	200	323	305	501	429	167	337
575	414	93	269	284	317	482	256	198	463	138
294	407	731	257	416	346	356	428	452	581	279
323	127	300	370	268	425	273	292	422	229	551
218	558	123	342	322	120	312	281	637	291	200
463	0	384	265	306	262	332	352	479	515	21
184	103	345	438	255	480	159	339	447	510	431
280	367	232	296	337	246	321	129	396	264	721
149	397	532	313	467	316	209	394	180	89	511
272	506	405	222	221	344	493	261	448	219	414
342	384	120	404	242	460	483	214	482	333	496
452	680	227	429	323	225	178	236	267	423	533
357	76	354	412	402	450	229	432	442	240	227
208	230	439	408	425	376	274	330	421	344	458
341	317	417	381	369	343	404	469	294	469	364
467	354	195	436	511	196	389	165	456	432	469
247	374	255	262	279	327	265	339	268	231	

277

1641.7_1164EK04	315	376	219	452	344	345	385	213	422	339
229	367	314	387	289	336	364	256	293	355	499
490	214	421	360	261	293	370	635	359	561	344
349	343	282	340	357	199	335	343	437	395	210
252	336	376	560	320	303	350	348	278	342	310
999	343	331	337	371	325	320	248	346	265	317
277	360	330	319	240	299	312	320	258	298	314
253	325	326	231	371	286	364	262	295	320	316
343	328	329	269	328	231	324	351	345	337	325
334	330	327	194	348	351	348	289	342	328	326
303	301	303	326	770	274	235	262	318	260	268
239	217	258	314	293	238	347	288	350	307	285
342	311	248	297	329	265	186	525	246	328	170
356	287	263	281	277	240	263	276	261	304	236
273	288	248	348	347	335	342	314	333	342	326
290	162	218	304	357	357	214	259	74	269	270
277	166	260	245	159	221	358	285	264	157	447
353	341	176	280	348	385	428	224	277	407	111
346	239	324	234	281	280	466	290	538	189	274
324	226	339	394	537	302	291	381	310	173	292
224	322	248	165	407	157	248	248	304	552	313
229	3	248	158	368	332	969	285	339	385	46
237	75	370	271	278	339	191	337	327	355	340
198	255	217	256	270	309	305	131	359	281	278
234	329	326	228	353	311	310	252	251	99	432
133	370	347	240	309	208	333	274	332	238	293
141	300	251	290	340	326	310	299	328	722	367
362	315	286	381	338	275	252	248	312	392	276
326	137	264	301	286	356	274	341	347	283	312
253	247	345	315	346	299	226	219	285	232	260
242	231	307	292	278	281	373	321	224	286	236
282	271	76	344	313	125	380	227	339	350	341
196	237	290	268	285	315	322	309	303	265	

278

1652.8_1288EC27	278	271	198	313	289	312	305	209	551	219
259	293	318	363	334	392	298	344	341	339	302
403	236	409	309	265	363	350	313	490	441	455
485	470	368	510	742	261	672	382	334	266	318
231	329	538	300	223	297	283	225	350	263	469
343	999	967	978	297	289	975	296	792	265	480
293	776	504	481	262	334	262	515	303	334	281
349	374	258	343	335	346	216	351	435	643	887
882	692	885	223	841	154	609	522	650	684	668
709	604	630	224	651	188	640	249	257	641	643
303	617	631	746	337	470	210	420	319	422	499
449	188	309	580	588	443	290	267	306	397	582
351	361	199	335	285	266	203	354	230	248	187
322	247	380	452	420	395	388	447	398	430	392
413	539	410	573	584	413	564	489	692	588	702
432	227	297	561	571	593	212	392	274	481	406
451	416	433	478	228	318	359	493	471	256	318
395	329	134	254	305	305	594	229	201	312	144
311	343	500	252	359	333	291	390	407	257	288
311	256	302	395	372	328	293	299	265	140	524
173	702	136	205	290	115	209	216	484	310	256
345	1	392	232	291	233	362	302	545	931	29
300	164	343	350	289	660	243	404	561	800	509
288	299	227	250	395	229	348	179	574	288	651
225	550	584	417	480	251	247	285	264	214	585
175	577	609	299	215	265	921	388	864	176	573
356	528	154	566	250	370	661	171	704	348	661
535	586	247	527	288	300	277	318	233	504	598
453	201	318	529	561	597	403	468	632	324	341
209	305	626	443	515	498	289	370	609	382	569
327	317	564	536	512	474	428	572	307	502	410
506	419	171	458	533	150	526	244	580	586	504
249	407	304	389	296	364	285	381	322	324	

279

1660.4_1288EC27	307	277	200	332	310	321	327	218	535	253
281	299	305	365	329	390	323	327	326	355	324
396	241	415	313	264	376	355	329	495	441	457
489	466	383	528	748	261	682	393	348	268	321
241	311	535	312	190	316	284	206	353	270	453
331	967	999	984	344	274	981	309	793	266	486
309	779	515	483	265	345	264	515	307	361	293
361	396	292	375	355	394	179	353	458	642	898
894	693	911	249	872	161	616	521	654	699	672
713	622	636	203	668	154	643	237	262	652	654
302	650	667	757	353	490	223	429	301	427	480
539	224	303	572	567	431	273	226	332	406	575
335	353	224	355	314	272	179	350	247	250	189
304	260	418	499	458	444	438	494	423	449	418
461	524	392	572	581	404	543	480	706	566	693
387	197	285	545	559	575	202	404	288	477	414
465	417	440	481	201	309	337	511	462	207	334
392	359	134	232	308	327	570	220	206	323	152
300	349	502	252	322	339	317	417	396	236	277
317	255	330	404	377	330	288	310	276	202	536
205	687	147	197	295	69	214	226	461	320	240
349	0	399	260	331	239	349	318	544	949	27
296	169	337	345	326	664	229	387	552	793	525
281	303	249	253	416	243	363	167	578	282	647
198	564	579	424	472	269	248	352	235	161	584
256	571	582	284	219	368	933	385	889	173	540
350	550	172	583	252	387	664	194	703	357	645
527	590	250	510	239	283	276	301	232	493	593
470	243	285	545	590	621	383	463	637	300	307
210	282	640	450	514	555	319	406	599	422	580
362	356	557	549	527	503	404	560	280	492	400
489	462	201	437	528	180	495	196	558	557	472
266	413	275	358	272	337	222	354	299	341	

280

1666.9_1288EC25	290	266	201	311	287	313	315	198	545	227
266	291	300	367	330	393	307	328	330	358	328
389	248	425	299	273	379	357	312	502	444	465
496	471	386	531	751	250	676	388	360	263	318
222	320	541	296	205	309	284	218	349	268	460
337	978	984	999	312	290	982	301	816	253	480
301	782	513	474	255	335	258	511	306	348	295
359	395	284	380	347	395	181	342	463	637	902
897	691	909	239	869	144	619	518	653	700	669
718	617	633	206	664	133	642	243	256	688	690
292	654	670	756	353	484	220	432	304	431	484
522	210	316	576	573	435	271	252	315	406	579
327	351	209	346	296	278	183	343	237	265	182
304	257	402	491	444	430	425	484	410	446	408
458	543	394	587	597	393	561	491	710	581	706
384	205	298	561	571	588	225	393	292	467	406
452	400	427	470	208	313	338	508	473	215	311
387	365	111	243	301	315	582	212	207	313	150
312	353	503	228	328	350	291	408	399	240	277
310	268	312	399	380	332	274	297	280	192	542
202	694	147	208	312	58	192	223	466	305	235
354	0	401	234	315	240	344	314	549	947	29
290	166	348	348	290	682	238	400	561	796	541
277	298	230	237	423	236	361	179	572	288	659
216	569	569	447	474	263	253	350	196	162	590
221	573	594	297	212	329	936	385	893	173	542
401	547	173	585	245	390	667	168	709	358	645
531	596	243	515	236	282	265	316	228	498	592
469	246	298	547	594	620	406	469	642	292	325
229	304	637	445	514	540	307	392	593	408	580
364	355	551	553	530	501	403	578	293	492	406
498	454	195	439	536	182	504	208	572	573	486
252	416	268	364	266	330	214	343	284	346	

1674.4_1164EK04	323	310	212	352	312	280	278	169	335	240
235	340	319	369	282	423	286	222	310	384	290
529	169	367	353	287	360	375	428	309	557	347
320	312	311	361	295	200	309	316	377	516	226
241	347	365	336	261	320	392	266	257	372	328
371	297	344	312	999	324	307	262	326	218	301
239	303	312	302	270	262	327	295	260	253	318
224	290	375	212	314	294	205	259	251	300	244
254	289	296	329	280	268	298	297	292	286	279
279	279	248	189	246	201	264	247	393	298	300
250	253	254	296	335	258	221	248	331	247	264
230	328	231	283	294	239	271	253	207	338	228
309	341	268	252	555	340	198	475	364	343	194
298	332	255	257	261	275	241	280	256	318	247
230	238	305	269	264	229	276	232	264	277	270
196	191	226	210	291	278	216	224	82	220	229
213	108	206	192	174	197	327	267	245	157	327
368	297	133	377	323	278	352	221	275	355	111
337	392	334	258	309	359	205	372	536	234	329
310	309	385	368	488	305	467	341	317	134	334
471	274	280	278	400	292	198	252	315	352	180
245	0	236	161	365	376	426	284	297	368	160
503	153	362	342	281	303	264	379	336	347	307
279	304	309	232	213	335	310	275	280	346	248
245	280	307	264	227	334	299	354	238	163	408
184	272	305	224	357	205	275	205	280	229	254
4	271	250	296	407	324	288	147	294	419	334
252	277	320	310	304	263	303	257	310	288	245
318	160	315	316	243	295	300	363	348	271	290
317	255	298	337	264	246	237	273	233	264	282
288	275	279	282	271	271	378	268	171	300	202
263	236	102	240	261	94	259	256	290	307	257
280	245	289	286	271	326	298	310	291	215	

282

1681.2_1164EK04	549	328	159	379	314	626	346	229	356	300
305	387	349	418	259	344	330	228	294	514	499
406	268	306	586	248	337	365	369	299	360	297
297	312	339	320	386	106	379	500	464	326	367
276	319	288	393	195	281	313	251	288	285	335
325	289	274	290	324	999	275	266	285	214	337
272	307	346	352	243	307	308	343	309	280	356
247	322	370	273	258	362	182	318	301	291	319
321	278	336	563	327	212	303	387	289	348	268
351	286	285	139	305	203	293	274	345	379	371
202	277	286	306	350	305	303	277	211	274	277
271	290	125	288	284	266	190	229	290	432	276
241	347	302	215	328	391	137	322	392	372	152
213	396	252	302	258	256	257	306	284	305	282
238	260	312	347	338	304	312	269	313	296	312
292	142	288	311	323	326	220	250	86	264	259
215	246	275	231	155	168	316	239	265	147	340
394	388	31	304	616	346	371	156	223	385	183
290	328	310	173	280	451	385	397	360	278	379
487	219	422	418	264	251	465	459	318	197	333
279	359	294	342	496	0	261	291	311	385	176
318	0	348	287	450	283	353	313	320	318	109
212	89	960	364	311	330	203	302	323	319	403
214	236	210	312	414	328	284	217	290	329	322
170	433	400	137	301	256	307	328	218	185	482
248	317	287	286	294	188	312	283	306	60	325
9	216	85	258	307	299	313	185	327	333	354
311	310	319	320	366	296	292	305	328	341	286
241	27	256	308	278	347	241	355	352	274	283
346	306	383	301	331	293	199	230	250	232	369
265	221	353	331	320	285	346	324	187	267	303
298	256	101	285	313	149	319	135	364	314	323
317	259	302	312	256	300	189	309	285	188	



283

1681.9_1288EC26	284	263	199	313	291	303	316	200	529	234
264	283	311	365	329	390	310	329	326	348	309
380	236	414	306	257	377	366	309	491	435	458
487	467	380	531	744	275	678	385	345	252	310
219	316	529	294	192	295	277	204	348	262	456
320	975	981	982	307	275	999	303	788	252	473
303	773	505	467	257	329	257	504	308	347	291
359	389	283	385	352	390	183	337	452	633	888
883	687	900	226	858	149	608	517	643	692	664
709	606	624	214	651	166	633	241	255	648	649
282	615	632	752	350	479	211	421	298	424	480
521	212	296	567	563	429	272	246	317	403	574
329	355	209	329	303	277	186	344	230	258	183
300	262	402	492	443	427	424	481	407	445	406
457	519	378	565	574	389	535	471	701	564	687
373	205	287	542	552	572	214	389	284	461	402
447	398	424	467	210	311	341	506	458	217	317
393	365	114	242	291	316	567	213	211	304	154
322	354	513	245	327	331	287	404	391	232	284
316	267	307	392	372	328	280	293	271	165	545
184	697	151	195	297	60	189	220	460	304	219
353	0	399	244	321	235	337	307	555	932	27
302	165	339	342	321	660	227	383	553	788	522
274	322	220	244	419	239	363	175	576	278	646
218	565	566	418	468	269	253	343	250	151	578
223	566	579	286	214	350	924	385	884	183	533
388	529	181	562	247	381	658	167	697	353	638
524	584	248	509	239	284	276	305	227	495	585
466	244	294	528	558	604	401	462	641	294	326
226	295	629	444	502	539	312	388	584	406	574
356	354	553	549	525	501	404	557	276	491	398
475	445	190	435	520	168	501	210	551	553	469
266	407	275	362	275	335	222	345	285	347	

1708.9_1344EC71	223	252	193	217	279	231	267	651	371	274
286	254	355	345	286	275	241	344	281	303	195
309	220	329	319	279	329	343	244	309	313	314
305	305	285	305	355	214	378	301	259	282	266
243	357	289	234	168	346	280	304	289	328	300
248	296	309	301	262	266	303	999	327	765	202
924	337	250	206	746	634	304	235	369	707	281
613	283	305	358	265	402	278	282	282	335	312
321	289	320	202	336	219	303	360	297	334	299
327	285	255	233	258	252	258	303	290	320	320
316	292	297	328	215	306	213	327	289	322	300
287	249	198	337	333	289	364	336	330	364	317
320	304	242	250	241	315	166	281	216	209	203
372	263	490	542	497	499	497	540	509	572	510
513	296	312	308	313	277	322	296	320	330	322
295	161	188	287	332	318	288	276	206	309	287
300	213	248	299	260	259	370	320	324	189	256
284	319	232	303	224	267	357	655	203	244	187
336	214	264	312	339	286	166	297	326	302	288
246	264	253	311	270	317	346	340	308	146	325
243	362	247	221	276	175	234	288	300	208	125
300	157	307	281	312	269	253	370	286	317	133
305	353	288	272	289	359	258	327	308	327	560
328	267	343	269	314	308	717	293	281	289	307
249	369	333	254	273	669	310	319	346	201	369
304	332	318	261	285	311	315	269	326	247	298
182	275	197	307	301	369	305	223	318	240	327
316	339	316	329	590	287	304	278	330	323	342
500	458	297	341	294	348	265	346	392	314	295
181	320	370	326	296	583	402	508	288	532	361
418	509	333	324	329	565	439	347	252	335	522
310	543	471	293	322	143	332	230	326	337	269
464	431	470	510	434	500	352	457	460	347	

285

1710.0_1288EC37	291	249	8	333	318	273	354	251	647	247
	252	327	276	315	350	421	295	329	339	381
	457	229	468	261	218	398	294	354	502	447
	487	485	431	483	827	6	713	356	358	297
	297	292	590	347	184	319	301	210	301	284
	346	792	793	816	326	285	788	327	999	268
	333	930	474	472	266	420	264	475	325	399
	380	422	245	407	346	450	197	412	469	648
	819	684	803	286	822	112	724	631	743	803
	802	724	748	32	761	152	751	231	255	768
	342	750	767	874	363	473	260	502	345	509
	466	260	303	688	652	434	282	220	326	372
	338	331	274	340	294	151	32	373	289	288
	302	167	462	522	474	451	469	512	453	461
	486	646	428	653	669	443	640	565	763	649
	457	10	299	654	611	619	209	436	309	478
	422	410	479	509	9	308	309	510	546	12
	331	384	139	203	257	354	667	217	176	321
	283	418	488	159	333	332	390	395	441	275
	254	133	239	357	352	333	264	275	306	189
	243	738	248	238	280	58	297	254	560	327
	382	0	415	240	332	260	362	309	609	780
	206	164	348	376	270	800	181	448	618	942
	307	411	319	208	407	199	351	109	685	269
	162	550	706	514	565	262	228	402	167	192
	247	668	654	284	199	239	850	437	846	113
	415	625	118	664	278	425	823	219	840	396
	625	685	172	647	350	247	149	307	248	620
	485	243	335	661	701	725	453	532	682	280
	190	300	680	556	612	631	333	451	648	464
	435	363	608	618	605	520	429	665	333	498
	568	489	202	420	615	176	591	155	619	629
	318	445	258	319	280	293	221	330	257	294

286

1719.5_1344EC71	249	245	209	226	249	222	285	578	329	217
289	239	288	324	278	310	255	304	219	299	223
274	224	311	287	290	297	282	241	317	290	311
313	322	252	306	297	209	303	273	218	232	254
197	308	282	223	192	369	237	223	281	251	245
265	265	266	253	218	214	252	765	268	999	266
803	270	293	262	853	622	269	240	371	674	241
650	290	280	297	244	384	197	293	285	301	264
277	265	253	170	277	175	299	307	288	307	259
299	276	272	206	270	225	286	269	255	281	279
257	259	260	273	256	322	259	304	252	314	218
281	195	234	250	244	244	300	280	314	338	251
240	283	221	226	215	267	165	222	222	184	204
292	250	515	588	525	521	503	562	521	535	511
482	231	172	268	280	233	252	236	257	280	253
211	131	161	251	269	253	284	252	106	269	259
279	81	260	240	210	223	323	303	263	142	239
277	355	242	230	223	285	311	580	194	256	272
295	238	238	277	291	279	171	337	294	237	292
294	236	274	352	274	283	303	335	307	110	309
196	271	222	207	231	143	173	262	255	240	142
270	177	220	306	303	193	253	417	253	270	46
246	287	233	253	228	255	243	239	265	272	553
210	235	337	230	309	256	662	220	244	248	221
190	384	223	171	234	731	285	302	244	149	340
228	282	288	248	257	281	255	264	248	204	290
220	213	183	274	258	333	236	180	263	270	292
276	236	289	281	561	250	220	258	277	286	240
526	463	225	260	243	236	187	230	305	249	238
87	282	275	292	269	602	411	530	269	532	322
410	455	271	286	307	528	358	278	134	245	527
233	541	486	262	271	156	268	207	262	244	239
487	387	387	417	342	382	327	367	348	244	

287

1722.2_1288EC39	363	273	193	243	260	323	275	210	533	162
245	503	309	363	312	347	278	283	294	336	363
481	296	639	337	259	400	347	323	561	331	531
576	565	360	381	516	245	488	367	390	304	272
248	334	440	269	189	281	247	230	322	264	417
317	480	486	480	301	337	473	202	471	266	999
239	475	946	969	258	280	281	931	295	297	283
275	342	288	320	363	318	166	279	359	428	424
427	425	432	291	418	171	483	455	468	439	432
434	469	462	228	466	167	458	207	243	468	456
313	418	420	443	285	437	255	438	306	430	402
404	263	313	447	439	335	256	206	256	397	369
338	327	192	355	353	267	198	352	240	258	177
277	282	331	314	333	340	310	349	323	420	301
284	349	290	505	508	252	483	378	463	462	471
235	216	451	405	488	473	228	282	203	244	294
257	332	231	300	216	270	303	339	381	230	256
361	297	171	249	295	275	537	219	197	493	149
276	341	391	240	346	331	293	603	504	329	353
416	244	506	582	256	306	301	349	355	89	410
247	555	230	227	409	21	217	203	416	320	141
334	0	355	231	347	240	328	288	506	528	27
248	130	367	429	248	462	239	319	614	481	421
280	327	253	254	344	248	343	204	372	289	416
211	427	418	304	394	291	257	393	223	245	522
237	464	461	447	213	256	448	382	426	147	418
399	430	169	434	227	339	458	154	464	293	482
425	441	238	397	286	356	227	450	257	391	384
399	190	279	384	397	408	291	393	408	356	390
222	434	414	358	425	338	286	317	360	305	550
312	263	349	384	360	319	421	421	181	374	310
405	366	207	433	404	90	449	167	513	501	382
232	361	299	340	330	358	231	359	308	307	

1723.3_1344EC71	258	242	223	209	303	234	318	617	372	316
282	239	334	317	248	272	311	323	227	318	215
316	217	327	348	265	322	349	238	308	327	288
304	311	268	284	348	225	349	297	231	270	282
246	340	257	237	173	341	289	302	269	332	252
277	293	309	301	239	272	303	924	333	803	239
999	337	268	237	787	617	286	250	336	678	308
604	268	271	348	254	387	234	269	263	318	302
319	298	309	217	329	175	309	357	301	330	282
328	290	264	259	264	225	284	311	292	306	307
303	301	305	336	228	315	227	300	270	298	268
299	225	182	318	321	279	323	325	316	332	302
297	274	227	217	233	304	191	258	218	234	201
330	274	496	546	518	515	497	554	525	530	507
484	256	298	297	306	271	293	259	317	305	310
289	174	182	261	299	294	262	258	186	286	260
310	211	245	274	266	257	357	291	284	204	263
273	312	222	274	242	318	350	624	267	255	193
308	218	242	287	328	292	179	313	304	223	326
254	249	248	310	273	291	332	334	300	141	305
277	334	251	237	263	175	230	315	246	219	133
282	156	301	277	293	260	265	370	286	322	114
305	303	284	263	301	355	288	302	296	333	554
265	266	317	257	317	277	678	300	279	297	256
243	364	290	216	254	654	267	327	339	152	375
270	325	306	256	277	294	325	290	333	204	302
177	275	183	288	298	320	282	198	313	246	332
312	333	326	302	569	268	282	255	296	307	296
506	442	282	316	286	310	245	326	384	291	286
170	299	350	268	305	575	396	499	275	531	332
400	471	289	304	314	564	396	323	221	308	484
266	528	487	281	307	190	289	212	300	303	282
445	404	444	487	396	454	335	418	421	311	

289

1726.6_1135EC25	319	291	99	338	328	299	325	232	700	237
273	353	303	351	454	491	272	336	389	352	381
471	252	517	303	226	445	316	344	589	435	545
575	563	444	520	878	120	750	365	352	286	304
313	319	617	340	199	366	277	218	263	297	517
360	776	779	782	303	307	773	337	930	270	475
337	999	513	486	266	406	288	504	386	407	281
372	485	245	415	375	458	216	419	482	680	797
791	723	812	309	789	142	756	664	778	800	684
801	752	785	107	813	179	796	231	267	786	788
347	787	801	881	370	476	236	516	338	522	556
435	262	281	706	677	418	302	205	351	376	587
351	341	279	332	296	154	122	385	269	247	210
315	186	436	495	455	427	458	481	443	464	432
458	604	407	657	676	418	650	541	740	655	725
426	120	325	670	626	633	189	437	289	443	448
402	393	450	497	135	307	312	509	535	146	377
391	394	111	194	274	325	718	215	162	374	137
277	490	526	230	371	357	399	407	475	265	293
277	145	254	382	324	402	313	300	399	143	522
242	821	249	253	308	59	317	268	584	334	210
393	0	430	284	312	216	386	311	677	772	47
220	153	352	440	268	796	196	435	621	980	592
326	391	295	242	412	235	377	113	612	275	626
165	539	700	503	555	311	195	422	185	206	643
280	695	667	328	200	287	820	397	792	152	697
410	648	127	677	247	432	845	223	860	389	727
651	697	187	664	370	280	169	362	209	639	590
437	246	387	691	721	754	466	552	687	291	261
199	342	666	566	657	591	309	422	607	492	621
459	357	589	623	617	514	496	642	306	538	436
544	451	206	469	602	185	600	176	636	635	598
310	447	266	348	292	337	235	355	266	317	

1730.5_1288EC39	352	280	204	303	311	346	279	234	565	194
304	490	301	348	354	366	266	335	307	321	333
490	274	621	324	259	408	356	333	593	340	589
608	596	384	425	534	244	485	385	408	313	316
262	328	468	240	227	350	275	263	355	263	426
330	504	515	513	312	346	505	250	474	293	946
268	513	999	936	288	265	290	948	320	286	269
276	346	290	352	380	346	215	334	378	447	434
441	452	443	211	429	193	539	473	526	480	459
476	527	514	242	510	219	511	246	247	472	458
339	473	477	476	319	475	230	491	309	484	409
417	293	346	468	463	345	291	237	287	395	386
350	375	255	390	358	282	240	349	269	297	195
330	282	327	337	352	343	339	393	338	415	314
303	370	347	508	510	309	481	381	468	480	476
298	240	435	408	513	510	258	316	200	296	321
310	325	286	307	265	293	353	371	380	298	308
376	237	197	211	320	279	581	219	143	502	137
255	346	396	244	387	306	267	590	506	256	335
432	189	517	574	285	340	306	363	367	200	452
298	590	220	200	422	109	257	201	443	304	203
351	0	372	258	325	232	344	315	539	540	29
281	109	362	436	276	453	242	313	583	520	421
309	294	205	278	386	240	358	150	388	279	415
217	465	477	266	414	247	240	403	240	191	533
250	506	526	446	215	177	451	376	425	195	461
406	484	155	493	223	347	493	178	519	310	512
463	492	229	459	284	384	237	440	301	452	395
374	52	306	448	460	454	321	390	440	396	400
230	431	417	443	461	360	278	310	402	346	545
313	308	370	409	393	358	458	429	255	381	341
392	363	162	468	396	104	486	236	507	514	394
253	361	356	383	370	387	315	391	363	302	



1731.6_1288EC30	364	271	185	242	269	328	272	208	545	153
241	518	307	369	316	353	272	287	298	342	359
486	293	653	335	264	399	344	323	567	336	541
584	574	370	388	524	237	492	367	387	303	272
253	338	453	269	197	285	255	225	320	273	425
319	481	483	474	302	352	467	206	472	262	969
237	486	936	999	251	281	288	948	298	300	288
274	346	271	311	367	324	174	286	366	437	430
435	434	439	293	428	178	483	462	469	445	442
440	469	456	247	467	167	453	211	243	474	461
321	424	428	459	291	427	251	447	315	441	400
406	240	318	457	442	341	258	212	252	406	379
342	333	195	367	352	260	215	347	254	274	179
277	280	328	322	331	337	310	349	321	420	308
288	356	299	510	514	263	493	388	477	485	486
241	235	459	435	517	497	230	294	211	249	306
264	350	237	314	235	266	304	352	391	253	258
368	300	174	248	303	272	548	218	192	507	143
276	349	394	242	347	336	288	610	508	338	356
393	247	489	567	257	311	304	347	373	93	421
246	573	229	229	401	21	216	204	423	317	150
352	0	362	231	349	239	329	305	518	531	27
249	127	376	435	253	471	243	326	624	488	429
279	287	252	253	360	251	349	214	378	289	422
203	440	420	306	413	295	245	394	207	248	539
240	480	469	453	214	251	454	382	432	157	428
393	429	165	432	228	342	464	161	467	298	481
440	449	235	404	280	361	228	456	261	401	410
403	188	284	388	405	418	298	390	415	363	399
228	438	422	355	436	340	282	309	366	299	556
321	267	355	389	365	318	431	436	191	378	315
413	369	209	432	429	86	455	166	526	512	393
237	368	311	345	335	362	233	362	309	305	

1731.7_1344EC71	211	230	206	254	265	207	306	570	309	275
313	261	302	316	249	259	281	286	196	308	208
297	211	302	299	281	289	301	246	300	303	277
314	315	242	296	288	195	288	278	240	277	280
246	327	245	205	171	368	256	228	274	291	244
240	262	265	255	270	243	257	746	266	853	258
787	266	288	251	999	601	295	231	351	677	262
601	288	314	305	242	405	188	263	275	330	257
260	254	240	153	250	172	298	280	284	271	243
253	276	263	212	267	230	275	288	309	252	251
243	260	264	277	241	322	223	277	251	291	231
278	200	241	264	259	260	256	311	302	332	235
247	273	256	243	240	288	182	281	241	225	166
257	299	530	581	549	545	510	576	546	534	509
498	227	201	265	275	219	263	232	259	314	257
225	150	167	230	280	263	281	276	110	277	271
276	23	266	239	215	162	320	308	272	160	280
285	298	258	275	204	306	309	575	245	246	256
314	187	241	244	282	250	188	310	326	246	257
296	259	291	350	293	257	321	366	279	14	291
245	252	264	235	275	191	209	289	259	215	111
272	195	237	330	307	246	256	403	240	289	61
268	305	258	211	257	230	217	275	255	281	523
231	247	338	249	303	296	677	228	221	276	195
207	373	247	139	231	656	314	333	240	166	318
227	307	310	232	307	235	260	230	251	183	279
225	268	191	264	304	322	254	175	283	249	294
279	235	327	275	542	230	239	258	320	264	246
547	460	240	259	230	260	209	263	320	231	198
171	275	312	282	249	587	424	561	248	534	302
423	486	259	321	314	536	356	279	98	248	554
224	558	497	239	255	162	238	204	268	259	255
485	400	372	387	332	388	320	361	366	235	

1735.8_1344EC63	264	283	185	282	261	260	262	594	404	237
233	242	288	312	311	403	234	342	346	312	244
348	264	383	253	309	326	306	282	344	340	329
347	337	345	373	385	246	398	303	256	252	292
210	295	361	248	179	338	273	312	285	262	348
299	334	345	335	262	307	329	634	420	622	280
617	406	265	281	601	999	251	309	370	709	270
634	369	235	380	325	429	265	303	330	326	357
341	281	342	204	376	226	333	364	327	443	271
435	321	336	267	347	297	338	228	249	461	456
305	290	297	350	335	265	199	370	331	365	320
273	195	218	324	308	307	332	257	284	401	371
311	324	256	254	267	264	238	277	219	220	239
340	229	546	583	562	542	556	592	535	534	551
572	371	340	385	391	379	367	372	385	391	393
353	241	271	332	365	361	289	297	203	324	301
361	255	324	292	303	287	381	337	382	266	300
313	368	216	209	257	262	414	602	168	253	149
278	406	304	277	413	300	232	335	376	228	293
248	212	249	308	275	396	371	322	356	216	357
184	391	336	254	294	105	213	233	320	256	156
381	109	363	212	323	270	311	336	333	347	186
308	369	306	265	338	460	255	378	306	420	742
330	289	270	317	308	272	717	255	358	314	288
144	422	357	225	345	630	241	327	351	227	438
268	373	353	316	222	268	356	300	365	272	383
192	304	209	320	252	484	307	224	328	352	447
359	345	241	345	652	347	242	348	242	357	384
559	454	234	344	305	369	158	318	399	353	335
190	350	325	372	349	665	392	548	307	592	322
490	535	432	323	365	545	498	442	307	370	569
400	589	399	320	427	187	401	300	377	386	369
529	495	446	521	437	453	361	470	426	367	

1737.0_1135ec00	299	320	199	339	343	338	359	218	299	264
265	292	693	362	231	324	341	192	318	346	336
365	207	316	582	288	322	597	388	307	361	306
314	334	230	252	275	258	315	425	337	376	272
253	667	360	246	176	273	323	254	346	788	270
312	262	264	258	327	308	257	304	264	269	281
286	288	290	288	295	251	999	283	208	262	292
250	235	519	280	247	285	194	322	222	255	234
243	259	264	338	264	197	286	307	299	279	268
282	297	301	208	281	181	286	689	556	273	271
238	236	236	249	320	244	182	264	259	265	273
226	226	189	292	303	285	244	775	264	375	237
286	304	229	210	319	552	197	278	263	295	172
256	489	236	232	247	250	249	266	290	308	244
206	252	234	248	240	233	261	228	253	263	270
251	189	245	215	267	248	200	224	114	214	235
237	171	209	253	197	205	292	229	232	203	315
325	269	68	785	309	359	324	194	215	325	173
728	303	281	257	251	301	206	313	357	258	315
299	557	317	375	298	288	420	386	261	193	267
287	319	196	174	364	222	260	491	334	275	155
226	0	294	250	354	332	317	395	255	289	29
242	93	335	262	310	290	262	303	317	294	326
220	280	374	327	266	635	329	414	245	311	260
640	309	301	163	258	275	471	265	283	172	325
211	260	333	250	651	201	248	206	240	141	272
0	233	168	303	532	255	244	152	257	331	294
236	337	733	286	244	259	390	238	744	286	248
286	23	784	303	246	435	576	543	465	264	280
220	222	390	266	280	245	152	232	241	261	323
241	255	252	329	324	286	345	246	94	280	274
243	238	111	238	234	185	250	110	297	292	240
248	236	271	279	272	300	234	289	273	241	

1745.0_1288EC30	377	281	194	261	295	328	256	203	576	141
267	484	316	349	343	350	239	320	285	326	343
491	277	646	319	253	380	348	319	595	360	574
605	594	366	403	544	242	487	371	391	308	282
256	305	453	258	206	326	275	233	317	271	414
320	515	515	511	295	343	504	235	475	240	931
250	504	948	948	231	309	283	999	310	299	275
269	350	266	323	365	337	197	286	361	449	457
465	457	461	225	456	188	508	474	495	464	458
458	492	487	251	494	201	485	224	228	489	476
330	461	466	456	310	443	227	479	311	472	388
402	256	342	449	433	336	274	232	275	396	370
337	357	209	388	316	266	229	347	252	269	190
290	269	305	338	311	321	305	353	310	407	313
308	366	334	534	536	272	503	387	495	508	504
273	270	455	447	522	520	276	330	190	269	335
316	330	263	319	276	287	314	363	394	285	279
359	279	189	224	309	256	581	229	143	487	130
269	345	399	243	378	316	273	587	509	284	341
387	217	480	549	275	340	302	333	359	106	441
286	598	238	192	425	11	236	194	449	319	154
368	0	377	237	313	228	329	277	550	553	23
257	109	353	439	261	472	250	312	591	498	434
291	285	252	255	365	231	368	185	367	296	407
195	442	440	304	415	259	218	381	181	208	545
257	497	496	444	209	201	478	379	441	188	450
387	465	149	472	213	334	482	162	491	314	488
453	464	212	426	305	377	232	460	257	413	382
386	201	301	426	461	452	311	378	433	378	412
219	441	444	403	462	357	260	282	385	289	543
305	291	375	417	397	344	455	448	216	384	326
413	373	178	453	435	75	474	184	526	525	403
242	366	315	348	343	361	253	370	308	307	

1759.0_1344EC20	289	293	278	247	253	273	290	326	447	188
237	259	336	356	504	438	260	347	630	336	312
305	235	309	252	277	424	302	251	432	289	463
420	461	413	450	363	301	405	284	295	277	341
295	229	417	279	230	459	274	210	236	225	362
258	303	307	306	260	309	308	369	325	371	295
336	386	320	298	351	370	208	310	999	362	346
387	347	233	514	345	513	176	322	354	372	336
329	367	341	308	383	205	380	333	376	332	358
333	380	369	319	377	266	374	143	263	376	375
258	359	359	359	284	272	207	449	260	448	382
268	186	177	370	333	311	206	181	288	312	246
276	257	240	223	247	247	344	251	182	191	274
259	208	319	323	327	320	307	347	333	412	318
316	321	345	331	328	293	332	299	327	313	321
295	369	263	318	332	322	217	251	217	259	256
238	289	251	278	358	170	404	287	299	378	266
398	464	169	165	254	290	463	316	166	319	141
332	455	361	278	465	350	304	419	304	285	261
297	190	272	356	218	568	322	278	479	214	440
183	401	250	286	353	114	285	251	348	302	167
441	0	402	265	251	235	291	267	398	377	156
270	164	349	451	317	402	264	317	407	368	395
279	380	262	357	360	213	369	176	309	356	404
115	392	419	250	267	368	164	502	248	222	410
305	341	356	337	187	238	360	239	360	188	337
0	379	184	356	256	494	367	206	396	294	358
319	377	255	300	401	350	248	346	244	326	290
298	193	280	416	389	443	146	378	404	335	315
153	335	375	366	307	391	274	294	265	340	376
299	338	370	370	357	336	453	329	263	399	396
312	303	134	371	333	150	308	279	335	361	247
371	328	383	428	389	412	355	426	353	336	

1770.0_1344EC63	245	276	229	304	296	214	255	635	455	233
281	284	272	282	322	424	251	252	348	282	251
351	255	381	226	273	364	309	302	368	358	337
345	342	341	350	408	252	387	265	283	248	384
265	262	351	251	190	358	325	211	287	257	313
298	334	361	348	253	280	347	707	399	674	297
678	407	286	300	677	709	262	299	362	999	271
721	328	224	344	282	457	204	370	325	332	336
340	374	333	207	322	152	364	385	352	363	349
363	335	333	254	354	276	345	193	205	379	379
290	329	333	379	304	308	180	344	302	347	301
288	234	262	339	333	304	264	288	333	320	344
276	254	240	258	248	149	208	277	267	283	200
273	152	604	670	628	608	627	654	607	608	654
582	339	308	333	351	334	314	319	352	358	355
318	189	243	328	343	340	286	296	197	298	285
376	315	297	299	238	292	316	406	311	240	312
319	349	234	196	219	255	453	640	154	294	103
258	424	317	330	255	304	233	339	363	203	248
269	136	219	309	305	364	265	264	391	152	330
201	377	201	257	284	136	283	221	343	274	175
321	241	332	271	231	200	305	309	368	378	43
237	320	262	283	197	395	165	290	293	399	573
203	352	373	300	236	189	977	112	383	231	267
140	374	434	243	292	778	174	366	216	179	404
241	371	361	294	165	276	366	248	333	201	349
177	292	208	345	218	388	351	170	365	339	378
360	376	186	310	524	297	143	281	228	344	379
548	521	189	324	329	371	141	371	368	303	268
215	322	310	352	361	631	455	608	449	641	334
574	554	335	360	368	656	452	376	181	335	628
318	617	508	302	353	94	312	149	328	306	323
478	494	347	384	313	367	347	355	315	319	

298

1782.6_1185EK08	312	310	208	436	368	272	344	222	317	317
301	340	272	411	354	319	354	380	311	360	396
398	270	340	355	278	323	315	319	287	419	287
300	288	327	289	284	195	344	402	307	352	351
621	328	347	291	228	430	419	245	298	348	277
314	281	293	295	318	356	291	281	283	241	283
308	281	269	288	262	270	292	275	346	271	999
219	250	343	330	241	301	180	358	282	284	258
267	278	269	371	302	205	285	298	301	306	265
308	299	271	247	284	225	272	223	525	325	329
268	263	261	271	322	242	314	271	261	271	276
228	310	159	265	257	218	217	240	240	336	245
281	309	298	245	426	334	246	365	325	298	251
245	409	247	280	273	257	235	287	255	316	267
262	262	295	305	289	295	312	271	294	287	310
291	231	277	278	325	293	223	238	185	200	244
257	249	217	208	272	198	338	287	265	253	408
371	394	194	238	314	344	349	216	290	307	202
271	309	322	244	443	356	302	313	381	216	391
336	330	295	374	356	281	438	370	303	487	284
352	333	256	402	324	152	624	395	305	293	175
272	0	283	261	372	427	336	348	330	302	173
349	137	376	272	353	350	532	369	313	304	302
219	315	265	356	309	337	307	256	286	974	202
209	357	292	203	246	268	279	284	283	320	471
186	260	378	262	397	191	281	181	261	154	340
4	274	170	252	519	312	256	220	271	318	368
250	277	322	282	220	325	274	296	275	304	267
314	144	301	346	303	311	213	317	354	339	306
313	287	327	323	296	316	224	289	264	257	314
296	218	302	395	420	295	416	339	185	300	320
285	284	152	264	306	209	268	135	306	298	271
255	237	355	408	373	365	265	352	310	260	



299

1813.4_1344EC13	294	248	237	286	296	227	317	571	380	234
	249	283	282	313	327	365	288	307	398	320
	303	309	330	243	268	357	298	281	361	267
	329	351	319	391	446	257	391	276	288	265
	250	252	304	277	194	340	257	225	285	231
	253	349	361	359	224	247	359	613	380	650
	604	372	276	274	601	634	250	269	387	721
	999	308	237	364	257	414	201	331	331	328
	388	323	373	201	374	182	317	384	306	404
	405	303	292	243	308	280	291	209	238	369
	259	339	344	377	255	270	218	321	259	325
	288	217	198	327	303	287	266	270	299	338
	265	247	267	252	228	157	204	258	236	226
	281	161	754	735	756	742	758	766	705	665
	665	277	268	315	331	315	302	274	338	337
	267	203	164	308	313	300	314	297	152	303
	321	193	323	282	231	273	289	382	307	241
	334	401	198	201	226	317	385	576	98	307
	281	295	325	264	327	358	215	370	320	230
	316	177	271	308	227	373	241	307	356	197
	182	443	174	263	245	126	279	222	323	267
	357	204	283	207	217	174	264	352	330	368
	200	346	241	324	231	390	130	333	346	382
	235	307	371	282	304	191	738	97	419	205
	133	354	322	320	286	906	202	387	205	127
	216	369	308	224	174	217	393	284	358	209
	174	284	196	309	215	353	353	175	364	297
	324	351	198	286	544	251	179	208	243	274
	589	580	203	337	316	297	139	293	313	258
	176	269	310	336	330	650	540	752	427	740
	676	606	385	298	339	746	375	350	279	313
	311	692	647	259	315	134	305	169	314	300
	499	571	335	359	311	400	290	334	308	230

1813.5_1313EC199	308	323	218	272	324	260	319	285	507	
243	270	336	319	312	379	379	278	276	413	390
652	307	265	331	238	281	450	345	232	455	319
429	455	459	339	424	544	283	504	287	378	298
267	221	276	421	328	270	332	315	221	278	292
391	325	374	396	395	290	322	389	283	422	290
342	268	485	346	346	288	369	235	350	347	328
250	308	999	218	342	280	377	216	315	499	438
407	419	434	414	369	418	184	429	718	438	463
425	467	432	448	285	449	245	445	191	230	536
538	243	412	413	420	280	343	212	403	274	404
360	323	194	177	362	410	363	218	223	321	314
387	272	275	245	259	252	151	272	268	291	256
253	256	187	340	355	338	340	329	344	324	404
339	354	349	288	518	546	340	498	394	545	506
507	312	284	207	482	510	513	263	320	219	359
338	309	397	328	356	296	187	351	276	385	295
286	403	341	165	190	239	319	508	294	193	327
91	296	352	439	301	352	374	734	293	287	281
274	290	173	275	326	196	424	334	266	387	202
401	168	553	193	263	364	0	217	199	402	316
254	297	110	336	261	330	271	302	218	680	412
181	276	207	334	384	196	414	242	252	388	472
445	298	331	335	293	298	208	344	111	327	270
334	146	427	381	305	646	356	172	307	261	172
459	287	694	366	246	197	325	409	512	353	212
291	541	349	152	400	205	405	446	232	455	253
451	697	477	221	637	394	278	214	261	239	641
424	280	252	279	421	380	457	244	397	369	292
224	164	257	386	432	643	403	275	344	317	320
345	531	314	326	379	394	345	415	392	205	339
377	397	410	222	554	430	157	538	247	492	522
650	288	357	341	347	319	316	348	373	316	250

301

1820.5_1185EK04	341	376	228	405	404	338	389	161	274	303
601	358	482	519	331	340	363	263	296	364	313
371	251	281	483	315	295	513	376	339	395	308
349	317	275	311	253	221	333	441	349	393	322
287	608	350	251	212	313	356	255	323	566	302
326	258	292	284	375	370	283	305	245	280	288
271	245	290	271	314	235	519	266	233	224	343
237	218	999	240	253	275	203	286	297	282	255
260	270	274	339	275	195	273	257	273	256	260
256	262	241	234	235	271	238	462	538	255	248
217	228	227	230	305	273	242	292	270	290	248
245	261	174	249	246	222	262	493	259	408	217
284	318	276	191	332	601	223	323	280	319	206
279	585	253	250	243	265	218	258	273	306	283
224	220	243	250	244	231	257	223	249	261	260
252	222	214	220	272	259	201	195	145	178	230
97	162	163	178	249	164	291	178	238	196	374
385	323	91	530	302	389	318	202	222	369	635
527	253	319	253	310	334	172	315	381	294	316
299	501	372	401	335	307	535	599	302	101	316
303	289	293	254	380	249	252	406	361	300	210
245	0	243	479	658	357	322	478	221	301	116
324	75	393	297	377	301	275	389	270	258	310
251	229	298	336	331	697	267	337	229	349	223
393	296	316	104	217	236	903	216	284	315	345
223	185	290	219	615	155	247	219	230	197	270
1	235	134	251	514	304	223	184	238	322	336
179	253	640	263	253	283	482	270	523	243	202
270	20	522	295	221	445	395	450	427	280	288
216	258	437	276	203	218	186	199	187	205	350
232	178	246	332	321	277	340	250	17	261	251
279	232	144	262	263	211	249	161	284	290	220
261	229	306	314	301	310	219	298	277	227	

302

1821.6_1288EC03	250	268	157	292	290	244	304	273	414	241
	220	285	231	320	493	374	282	482	432	329
	350	242	344	237	257	398	263	230	352	257
	360	376	466	433	444	210	412	288	237	254
	256	284	400	250	176	367	325	218	268	264
	231	343	375	380	212	273	385	358	407	297
	348	415	352	311	305	380	280	323	514	344
	364	342	240	999	280	793	185	424	397	427
	386	406	373	242	420	141	480	436	470	480
	491	469	449	237	430	188	430	217	265	474
	269	497	490	460	217	412	211	390	258	393
	377	235	191	472	461	364	239	217	248	370
	287	270	254	256	250	179	218	313	210	257
	273	199	351	402	379	388	374	421	383	461
	402	424	384	459	473	405	451	416	462	461
	368	250	281	474	461	483	239	298	153	313
	313	337	303	302	248	251	309	299	410	264
	385	345	142	225	229	304	426	234	135	289
	223	376	347	265	542	324	311	435	346	313
	291	165	308	318	190	395	274	276	464	153
	184	478	181	261	235	109	263	229	350	259
	458	0	476	226	273	291	245	299	440	404
	249	117	297	386	316	445	241	326	399	440
	291	409	234	288	311	211	414	141	385	345
	146	380	459	315	413	351	212	773	195	203
	284	518	414	296	176	243	397	314	354	187
	366	473	75	468	225	414	482	180	493	253
	460	464	235	438	315	264	234	327	257	460
	331	141	298	489	483	381	171	393	371	275
	157	316	333	370	441	413	268	381	383	401
	397	372	419	429	387	424	406	457	272	391
	400	402	207	404	448	159	424	248	464	446
	266	364	381	389	360	359	284	364	319	373

303

1821.6_2011EC49	340	329	162	279	279	289	299	247	447	185
232	314	301	354	439	461	246	245	464	318	282
364	230	394	282	219	368	314	321	472	306	438
462	472	339	437	411	200	381	267	312	322	271
251	278	451	267	230	378	296	277	254	246	476
371	335	355	347	314	258	352	265	346	244	363
254	375	380	367	242	325	247	365	345	282	241
257	280	253	280	999	389	226	306	345	387	306
315	361	337	336	342	192	401	353	399	313	357
338	398	382	209	403	225	400	225	238	371	390
516	341	340	351	338	317	208	367	632	368	353
300	273	398	390	366	323	329	225	387	285	351
509	348	228	467	300	199	211	288	240	197	195
373	226	302	308	322	331	293	339	335	397	328
324	288	241	320	287	353	279	252	344	319	358
275	239	207	285	292	309	250	402	220	438	407
410	352	424	419	213	328	371	458	272	236	296
394	508	221	207	262	299	437	235	162	336	93
259	436	427	257	363	278	274	375	399	283	228
379	183	284	347	215	448	283	253	386	253	414
152	394	187	209	308	109	278	212	363	298	261
325	160	273	226	278	244	363	273	323	344	55
274	215	273	335	308	365	186	313	362	369	374
211	354	258	278	261	258	325	163	272	275	322
150	361	313	257	280	285	162	290	270	134	323
198	330	327	213	221	263	322	231	292	251	287
174	309	202	329	231	419	351	193	363	332	339
281	390	229	283	270	245	174	238	203	290	353
299	179	270	375	302	322	116	340	337	284	225
220	241	326	353	337	305	303	282	259	332	334
231	311	246	289	269	349	424	242	275	356	243
246	303	210	267	278	161	285	213	271	265	262
245	256	321	324	336	384	359	382	348	206	

1826.9_1313EC200	312	331	237	314	297	294	327	342	451	
264	307	302	303	412	459	480	304	401	467	328
370	393	288	409	299	333	481	355	296	394	321
366	405	398	458	470	485	289	496	353	342	324
368	305	357	431	293	203	440	332	324	321	308
423	286	346	394	395	294	362	390	402	450	384
318	387	458	346	324	405	429	285	337	513	457
301	414	377	275	793	389	999	301	347	429	438
382	396	423	416	320	424	234	418	481	411	485
435	499	411	381	343	416	285	390	249	316	496
507	415	428	432	456	275	401	243	453	364	450
462	392	277	214	461	470	401	405	256	330	398
453	399	377	340	252	311	273	307	312	253	268
299	407	281	360	389	375	372	342	402	368	536
414	434	429	392	443	446	425	441	418	437	446
426	398	302	292	457	451	472	281	375	234	362
385	382	387	358	341	332	308	446	356	445	345
326	449	424	202	239	267	327	462	323	198	320
173	279	452	416	347	468	330	367	468	413	337
299	317	265	304	351	240	490	384	347	474	198
482	247	547	233	305	349	144	317	276	442	322
188	489	118	548	312	358	327	311	388	482	430
194	321	181	390	475	381	536	278	400	379	488
485	438	474	300	378	359	292	455	272	411	356
417	156	434	493	377	437	413	266	955	382	239
502	327	497	408	332	251	331	421	323	403	287
430	266	384	222	420	316	457	438	246	461	315
498	475	491	294	464	427	388	315	377	303	479
491	419	314	331	454	424	419	211	435	390	405
362	240	369	391	448	465	453	348	384	372	415
413	427	426	441	470	437	396	530	474	336	466
507	425	393	244	412	460	214	484	305	459	494
417	384	428	548	552	512	530	398	497	486	484

1843.5_2011EC47	210	294	187	195	196	219	205	184	225	129
195	210	194	216	174	208	191	184	200	275	221
270	199	298	208	173	192	191	220	209	240	193
215	185	195	232	248	220	240	226	187	260	179
197	184	215	248	222	285	204	609	237	189	197
364	216	179	181	205	182	183	278	197	197	166
234	216	215	174	188	265	194	197	176	204	180
201	216	203	185	226	301	999	152	248	253	190
187	190	189	156	189	313	184	208	184	213	203
215	179	171	211	182	352	191	209	199	225	253
283	188	189	205	239	170	207	208	268	207	175
160	198	222	173	177	160	255	170	325	248	234
261	337	297	238	217	224	198	200	254	219	182
292	203	206	292	229	241	240	281	290	349	259
230	167	185	168	169	338	174	188	227	244	225
316	187	235	178	183	188	243	232	50	243	257
197	93	238	171	181	118	312	248	202	169	190
251	268	244	135	214	205	215	166	120	224	102
159	69	259	177	215	170	171	211	283	139	215
167	214	202	205	230	199	221	246	153	127	184
176	240	169	127	210	205	184	169	199	231	215
199	264	216	160	248	184	368	192	189	202	37
235	96	201	167	219	205	196	205	180	209	272
203	120	209	208	181	217	173	148	191	209	115
155	222	136	163	230	174	193	198	361	155	231
204	175	210	231	208	226	188	162	189	240	215
139	140	281	178	204	209	187	208	197	228	214
185	190	214	204	196	301	199	242	191	185	189
180	6	101	240	174	161	147	144	181	323	269
184	243	183	238	204	165	258	130	194	202	146
147	193	187	218	205	254	291	198	188	188	173
151	220	86	161	214	161	162	194	181	161	184
199	140	314	318	269	338	288	303	285	229	

306

1853.9_1164EK02	287	273	166	175	196	288	335	275	410	233
	211	235	344	379	395	446	292	477	341	247
	298	289	337	339	233	383	354	259	355	307
	350	361	339	364	384	216	382	367	259	276
	266	357	386	215	198	351	326	197	202	354
	262	351	353	342	259	318	337	282	412	293
	269	419	334	286	263	303	322	286	322	370
	331	315	286	424	306	347	152	999	342	399
	428	408	423	215	412	220	439	444	441	448
	433	426	394	216	398	140	409	258	368	411
	197	418	414	397	226	301	219	386	233	385
	306	185	217	413	374	340	212	267	194	396
	230	291	218	235	257	307	191	239	198	197
	203	321	323	402	307	317	308	323	342	370
	343	379	296	411	395	339	362	341	360	350
	325	210	287	340	378	385	191	267	292	221
	280	207	211	264	194	280	312	314	353	216
	396	355	157	332	289	335	411	330	265	264
	333	415	375	255	473	290	193	368	351	331
	319	254	277	369	227	304	277	322	364	17
	161	448	132	260	309	32	261	323	384	246
	404	0	408	226	284	333	289	341	340	390
	277	121	338	374	201	419	431	301	389	442
	337	331	288	315	390	302	400	278	322	396
	243	396	343	271	306	317	266	282	182	349
	213	355	492	266	303	185	439	265	429	151
	0	397	200	445	333	395	416	187	427	280
	332	364	287	364	267	273	245	327	264	372
	355	308	344	469	442	453	306	404	450	280
	117	313	394	343	343	408	217	326	328	339
	369	337	393	457	445	418	433	410	264	375
	355	406	249	325	402	183	369	133	374	397
	258	356	313	354	286	366	220	345	318	325



307

1854.9_1164EK03	318	303	186	289	278	290	330	257	478	250
257	258	304	351	465	450	288	379	427	347	370
352	274	356	251	454	389	299	278	410	271	401
405	395	369	466	519	247	497	290	276	249	293
298	319	422	276	273	289	268	275	256	255	389
295	435	458	463	251	301	452	282	469	285	359
263	482	378	366	275	330	222	361	354	325	282
331	499	297	397	345	429	248	342	999	417	425
433	403	431	316	448	186	470	532	461	501	426
502	452	444	304	451	228	448	173	257	515	500
270	451	455	467	276	380	165	382	282	382	435
397	212	173	478	465	428	273	221	295	318	488
303	293	274	226	278	197	310	320	242	234	295
298	196	304	375	297	319	302	344	313	483	346
444	381	331	479	486	328	468	447	481	503	497
350	336	294	588	456	460	253	666	489	379	671
324	400	410	564	329	256	374	265	462	330	295
401	353	139	197	272	330	476	243	225	296	153
286	423	395	414	439	364	402	376	350	346	281
317	207	298	337	186	452	356	294	448	213	465
168	514	247	288	298	30	304	225	377	285	229
429	6	423	263	319	226	303	292	524	445	164
270	174	320	444	290	479	220	371	455	497	463
320	375	319	334	325	254	329	298	456	314	436
236	401	489	409	521	308	230	383	272	233	484
302	594	426	288	219	290	445	379	428	204	408
325	381	201	425	245	462	456	271	466	298	457
569	512	241	461	370	292	266	361	279	472	538
353	222	331	452	450	563	230	469	528	285	256
184	338	385	370	474	418	297	340	392	337	413
375	354	462	450	436	335	459	481	264	441	440
479	404	193	463	507	203	479	244	488	480	493
351	401	370	399	375	378	382	403	333	369	

308

1862.2_2011EC39	277	297	201	304	303	296	315	287	611	246
277	305	312	377	431	429	309	344	381	351	338
445	247	477	310	271	424	333	311	497	402	492
505	492	443	466	738	248	629	416	333	293	306
313	352	510	287	236	388	335	265	310	292	463
320	643	642	637	300	291	633	335	648	301	428
318	680	447	437	330	326	255	449	372	332	284
328	438	282	427	387	438	253	399	417	999	681
693	976	687	364	675	206	544	550	545	661	971
662	524	530	204	547	241	537	223	288	619	620
332	550	561	649	328	372	244	439	326	444	466
394	304	278	575	541	382	334	254	331	387	517
342	360	240	291	296	321	191	338	278	300	205
334	267	342	438	356	336	349	388	364	451	346
420	461	431	550	546	413	500	441	645	529	627
431	207	296	537	452	472	202	389	301	415	402
446	335	423	415	197	338	404	446	409	221	332
370	434	167	238	267	315	624	297	244	314	184
294	397	464	319	391	386	310	413	468	261	303
253	237	266	334	328	353	282	308	448	145	474
198	702	175	292	347	211	291	278	489	302	215
431	118	477	339	334	289	363	327	673	647	227
325	200	362	445	318	623	268	412	552	700	457
384	325	293	307	399	307	359	299	572	307	578
187	531	528	442	478	295	271	356	347	234	592
285	584	535	322	251	335	736	340	716	260	544
334	497	197	530	290	361	617	258	633	375	616
543	564	235	556	308	334	316	322	287	527	526
408	307	326	538	551	586	372	445	573	384	354
261	332	607	569	524	500	275	340	510	365	589
373	360	524	555	543	431	498	511	379	515	434
471	379	221	442	493	147	477	253	467	489	505
332	396	367	425	359	422	320	454	403	363	

309

1865.3_1135EC00	276	272	118	296	296	302	253	252	635	247
	268	300	280	364	370	406	284	306	398	313
	424	250	477	298	262	387	310	323	507	420
	495	484	396	478	832	181	730	360	265	255
	263	320	537	298	204	275	251	243	284	230
	316	887	898	902	244	319	888	312	834	264
	302	797	434	430	257	357	234	457	336	336
	384	407	255	374	306	382	190	403	425	681
	975	709	942	306	908	159	590	593	610	772
	771	572	587	129	613	112	612	203	229	716
	291	667	682	804	344	438	182	419	301	427
	451	197	275	617	589	392	248	218	259	378
	319	321	204	300	307	235	118	338	235	235
	285	233	385	465	397	372	412	437	407	425
	465	579	405	580	583	384	558	519	721	576
	415	143	283	603	529	543	167	378	255	439
	381	369	404	449	152	300	324	430	491	179
	396	337	135	195	274	253	646	264	232	313
	303	371	510	218	342	345	305	428	450	247
	230	221	241	342	324	362	266	286	381	185
	139	782	225	223	294	60	241	247	499	293
	377	0	401	226	292	217	332	290	636	915
	231	172	364	436	271	724	243	442	565	806
	347	348	202	254	460	236	374	175	646	277
	172	560	552	457	494	278	247	385	221	166
	227	610	581	301	200	319	966	353	921	147
	392	528	131	573	222	383	688	183	703	379
	561	621	225	527	353	249	258	298	223	495
	457	338	316	556	614	626	428	458	634	270
	247	294	597	476	552	547	265	368	637	436
	404	360	583	579	527	458	438	608	338	524
	521	453	246	380	571	139	475	229	541	539
	229	420	279	338	296	366	239	371	295	301

310

1866.7_1185EK18	287	299	180	306	306	311	259	267	628	245
263	310	285	383	376	453	290	330	384	329	328
431	252	488	296	265	387	320	334	518	432	495
506	498	389	512	825	216	727	387	275	259	278
292	315	546	310	219	301	268	248	296	234	480
343	882	894	897	254	321	883	321	819	277	427
319	791	441	435	260	341	243	465	329	340	267
388	419	260	386	315	396	187	428	433	693	975
999	724	941	303	933	160	594	593	615	785	690
771	578	591	160	618	180	621	195	241	693	694
285	653	667	788	357	443	171	426	303	432	478
454	202	281	640	608	426	237	199	284	379	572
322	345	213	299	289	249	151	322	233	241	175
269	210	388	485	402	377	414	445	406	434	377
473	580	406	577	579	393	557	517	701	572	711
427	172	305	591	529	537	218	377	256	433	383
372	374	400	439	197	317	321	430	488	201	331
404	361	176	181	280	259	643	277	236	324	158
299	424	520	243	342	349	297	378	453	259	283
238	181	261	356	332	366	280	310	388	206	518
142	781	193	260	298	26	256	281	491	313	200
360	0	414	228	298	240	339	311	641	911	39
276	175	371	443	277	717	246	446	595	799	525
333	349	229	254	449	220	380	124	640	273	701
158	565	578	465	483	285	243	391	216	141	625
231	605	567	318	212	379	960	349	930	186	586
375	521	136	574	230	396	685	200	697	392	704
556	635	197	526	314	296	242	334	230	495	550
458	342	314	555	621	627	431	479	646	322	336
237	328	637	469	545	569	288	372	631	443	603
404	344	590	564	532	477	461	609	333	530	414
519	446	243	381	565	88	476	208	542	543	524
229	441	293	357	320	361	255	375	279	327	

1869.2_1344EC16	300	291	140	311	311	295	326	240	655	208
268	310	302	381	434	489	319	323	404	375	337
433	259	491	309	262	420	321	318	538	410	527
524	515	381	464	759	157	655	421	306	275	291
323	329	490	291	219	390	289	226	308	255	447
328	692	693	691	289	278	687	289	684	265	425
298	723	452	434	254	281	259	457	367	374	278
323	434	270	406	361	423	190	408	403	976	709
724	999	712	374	726	159	575	553	572	675	975
675	553	583	115	598	125	593	200	252	632	632
314	545	555	658	321	363	228	443	269	444	420
396	269	251	545	500	353	227	219	280	372	525
301	324	246	277	267	298	107	304	265	284	163
249	262	379	486	387	377	408	454	417	440	312
433	495	414	540	549	394	528	477	672	553	666
381	112	291	526	484	497	158	379	271	411	397
407	335	398	437	119	324	332	415	438	134	335
387	440	148	212	268	326	659	254	190	334	151
294	451	483	256	352	397	294	403	453	249	307
280	191	240	350	314	386	266	311	415	138	478
204	726	128	292	326	27	289	296	476	307	193
400	0	444	306	306	240	338	291	683	697	246
269	145	340	425	277	677	236	404	596	726	489
361	348	257	295	379	273	400	159	615	293	634
158	549	527	492	466	283	217	429	229	199	578
271	582	510	303	226	318	762	322	740	150	512
318	483	152	507	243	437	631	177	654	356	627
536	576	212	505	284	257	305	335	263	449	526
420	263	313	516	541	567	388	443	586	286	265
230	331	610	528	515	515	268	339	543	395	619
401	419	551	518	503	467	485	564	306	507	369
506	346	237	463	513	101	482	226	500	516	497
263	411	290	346	310	389	247	388	313	307	

1870.1_1135EC00	288	279	134	332	325	296	290	229	625	235
	275	310	311	378	401	430	303	312	420	340
	437	256	473	311	248	397	340	324	510	452
	496	485	405	502	822	173	719	373	310	266
	288	326	551	325	192	342	283	218	346	253
	329	885	911	909	296	336	900	320	803	253
	309	812	443	439	240	342	264	461	341	333
	373	414	274	373	337	416	189	423	431	687
	941	712	999	280	964	147	601	595	619	781
	764	585	604	149	637	125	620	218	253	682
	289	634	647	807	353	467	181	448	324	455
	413	204	293	608	582	404	269	213	287	390
	340	334	246	315	312	249	133	357	244	254
	289	234	415	494	434	406	417	452	419	450
	445	554	425	547	557	407	555	500	737	569
	442	147	262	603	519	530	181	393	312	503
	454	440	473	525	157	362	319	506	469	161
	411	357	105	221	290	290	639	248	204	334
	294	423	503	227	354	366	319	406	455	239
	265	240	237	348	368	382	268	318	364	156
	205	799	180	244	278	62	258	251	500	332
	397	0	395	229	300	214	352	321	625	906
	242	168	381	396	290	703	220	433	576	818
	347	354	217	249	439	247	365	171	608	266
	184	532	591	466	503	293	229	408	236	174
	216	626	558	285	212	295	945	344	954	164
	392	496	149	533	225	372	695	198	717	380
	587	620	246	541	321	255	284	285	226	511
	447	256	325	553	572	633	405	487	655	265
	237	281	627	456	550	584	273	389	613	448
	416	343	586	588	545	472	436	607	320	536
	497	452	243	394	550	140	482	220	532	533
	260	453	266	342	298	381	219	358	298	308

313

1871.6_1164EK04	312	246	3	267	273	260	292	148	296	229
	219	285	387	302	349	412	340	203	363	439
	331	120	292	362	265	328	411	346	316	350
	341	338	324	364	311	2	292	303	466	353
	240	350	367	307	142	364	329	174	290	329
	269	223	249	239	329	563	226	202	286	170
	217	309	211	293	153	204	338	225	308	207
	201	369	339	242	336	320	156	215	316	364
	303	374	280	999	284	103	294	279	297	229
	234	277	255	3	257	156	261	177	343	252
	195	278	278	299	287	322	281	306	149	308
	232	317	180	237	276	246	137	247	244	380
	158	244	228	239	392	319	5	395	360	372
	172	253	206	241	207	209	203	242	283	291
	265	247	286	254	240	220	275	234	259	256
	248	3	131	215	251	233	153	319	131	263
	275	220	293	269	7	129	226	262	197	3
	462	407	1	255	308	292	278	92	243	327
	321	380	339	296	243	655	275	224	313	232
	342	62	274	330	308	352	288	319	362	207
	359	305	188	515	469	0	229	236	332	260
	276	0	246	234	336	287	302	378	362	284
	103	43	564	286	276	228	272	322	313	319
	229	317	235	242	244	303	277	78	277	369
	127	304	262	308	276	242	264	351	107	106
	179	336	235	195	269	281	302	178	280	1
	29	215	1	312	311	342	310	247	318	366
	309	332	301	343	218	105	259	101	323	365
	252	153	334	294	287	336	121	308	323	146
	311	102	348	325	332	257	159	231	219	214
	286	273	226	321	288	275	320	258	129	279
	258	200	5	340	242	208	288	5	264	290
	176	238	175	174	177	222	214	213	176	189

314

1875.4_1185EK18	294	325	146	303	289	300	278	269	625	256
272	313	302	395	380	445	292	310	407	348	348
425	242	490	332	259	426	345	349	539	454	515
541	535	410	490	805	180	712	407	300	299	291
306	333	544	302	220	354	284	237	319	262	477
328	841	872	869	280	327	858	336	822	277	418
329	789	429	428	250	376	264	456	383	322	302
374	418	275	420	342	424	189	412	448	675	908
933	726	964	284	999	175	603	608	620	774	698
752	586	601	126	628	102	627	213	256	696	699
294	615	627	784	344	453	185	473	297	480	490
457	246	235	645	612	417	223	181	273	388	573
311	356	237	262	313	257	118	355	235	243	130
258	245	403	498	418	395	420	439	401	448	393
482	553	428	576	584	416	571	511	731	577	744
422	122	258	583	530	536	197	378	251	425	378
347	360	404	448	132	307	304	415	469	145	333
415	361	172	209	274	278	642	269	245	356	156
309	432	505	237	364	368	302	420	457	247	293
279	198	245	372	345	374	291	331	422	176	498
182	786	237	282	319	26	271	286	493	304	204
431	0	402	246	307	254	320	328	639	889	144
274	198	372	450	306	738	227	435	577	797	541
347	375	245	273	440	237	379	144	694	310	677
171	552	571	447	486	278	245	425	222	171	636
233	615	554	289	234	295	910	348	952	137	591
386	490	138	528	241	422	690	183	704	375	691
564	673	240	527	331	249	238	284	242	498	559
450	337	312	562	576	633	427	484	677	295	302
219	278	680	451	551	597	273	381	613	451	622
423	376	597	573	521	485	463	611	322	536	421
519	465	268	383	553	92	477	261	543	552	527
257	461	284	344	294	363	247	373	272	310	



1879.6_1344EC04	227	237	284	189	186	218	203	166	152	163
207	209	227	213	250	209	213	237	145	208	188
215	179	184	210	197	154	242	282	167	250	137
168	155	167	225	154	318	201	210	187	255	227
193	213	129	225	131	234	220	261	139	238	218
231	154	161	144	268	212	149	219	112	175	171
175	142	193	178	172	226	197	188	205	152	205
182	184	195	141	192	234	313	220	186	206	159
160	159	147	103	175	999	114	154	115	163	148
176	137	134	294	144	351	141	243	197	160	176
230	111	111	113	261	140	166	140	230	127	125
185	181	175	139	129	159	255	153	275	240	191
281	226	328	208	189	261	299	201	223	47	182
288	213	194	204	216	212	203	242	232	265	236
219	179	170	158	161	364	147	208	178	186	187
298	288	215	144	138	137	233	143	155	135	238
186	89	218	130	297	154	268	225	185	287	217
217	179	172	175	223	203	131	190	210	233	273
209	138	141	253	159	165	95	127	206	161	257
126	175	225	164	240	236	275	238	178	192	182
66	166	160	181	176	233	195	221	143	221	109
213	170	156	196	214	188	276	161	139	156	24
182	103	220	143	130	123	221	170	127	107	219
215	145	190	287	129	231	110	55	143	240	106
124	163	115	164	178	71	215	107	376	246	188
136	169	167	202	248	153	124	137	131	676	190
129	169	223	146	257	140	122	197	117	239	150
164	146	236	157	85	294	269	222	208	144	209
155	196	122	181	103	124	94	128	146	333	303
144	222	144	199	141	163	258	183	208	135	141
129	147	198	141	165	198	245	156	141	159	146
183	179	50	123	233	215	113	259	149	129	150
247	92	279	306	245	231	289	253	254	209	

316

1879.8_1185EK17	309	322	194	335	322	305	355	251	653	292
285	345	320	371	416	456	335	339	400	367	379
434	259	476	279	273	442	330	306	640	376	627
654	662	410	477	678	254	617	356	377	324	342
333	322	549	338	196	347	339	206	276	318	455
324	609	616	619	298	303	608	303	724	299	483
309	756	539	483	298	333	286	508	380	364	285
317	429	273	480	401	418	184	439	470	544	590
594	575	601	294	603	114	999	584	970	641	555
660	982	969	242	905	156	940	218	292	643	642
313	812	801	758	323	434	240	529	268	511	579
413	345	244	665	634	340	272	203	311	396	529
325	369	269	284	303	248	209	309	292	260	233
277	269	446	493	461	441	463	465	441	452	382
439	519	342	680	668	366	648	466	629	636	623
359	248	337	597	601	599	207	360	190	342	369
341	309	335	371	258	187	330	396	468	277	350
417	476	171	208	305	355	671	233	273	360	129
297	447	476	231	393	349	342	406	416	257	281
389	202	423	483	264	418	306	317	397	200	468
237	709	150	255	324	23	323	247	532	286	223
396	0	408	230	342	261	317	337	611	619	28
314	124	355	396	304	658	257	390	542	759	476
349	378	268	259	421	206	378	106	530	296	506
184	510	605	440	527	283	198	409	268	204	591
305	584	679	338	218	316	600	349	575	109	690
346	921	161	915	254	428	839	245	838	340	630
563	654	244	702	311	306	264	358	245	697	556
459	214	301	778	847	672	342	491	560	327	350
217	356	521	516	559	501	320	440	491	485	617
421	397	488	520	482	475	474	546	257	458	411
470	448	243	511	526	148	576	180	604	591	581
269	417	314	388	281	372	244	395	316	350	

1879.9_1344EC77	315	353	157	326	341	332	305	273	647	232
295	382	331	326	389	414	274	360	401	401	561
405	260	450	279	245	476	377	315	503	427	471
516	531	432	486	714	193	643	386	403	303	344
276	307	546	353	218	417	374	257	297	346	446
351	522	521	518	297	387	517	360	631	307	455
357	664	473	462	280	364	307	474	333	385	298
384	718	257	436	353	481	208	444	532	550	593
593	553	595	279	608	154	584	999	601	646	537
648	589	621	211	615	177	606	245	315	669	669
328	561	567	592	314	464	271	485	336	490	500
447	260	279	541	546	424	286	258	354	387	507
327	362	241	319	275	170	223	268	338	303	255
305	209	417	472	433	409	432	470	425	461	432
449	500	417	663	691	407	625	513	676	632	658
441	235	280	605	636	643	239	406	218	384	398
369	375	357	400	243	228	352	398	511	253	342
432	426	153	177	306	305	658	244	144	400	150
294	405	462	246	394	330	558	423	381	317	269
295	140	297	401	300	414	305	369	428	274	494
268	738	105	265	340	13	277	264	504	323	283
410	0	409	287	398	301	345	307	695	581	109
230	197	402	395	318	609	197	360	492	690	563
355	305	290	265	425	230	421	124	510	303	515
140	502	600	357	716	359	234	394	203	196	605
295	803	574	303	194	229	605	746	546	144	491
469	515	187	545	253	479	621	187	634	356	653
800	611	233	756	393	280	198	350	283	753	575
399	134	253	558	556	638	341	478	586	317	251
236	350	560	499	752	568	252	409	486	427	503
571	378	522	487	490	510	502	559	259	452	426
518	488	163	533	560	136	686	184	651	663	747
347	456	335	345	331	389	243	395	320	291	

1883.7_1185EK19	318	328	188	347	333	301	340	229	656	286
293	355	325	376	409	470	336	340	406	373	378
449	254	490	290	276	429	348	326	638	382	628
652	663	405	475	707	245	640	354	362	315	342
342	315	525	325	197	346	345	202	283	311	461
345	650	654	653	292	289	643	297	743	288	468
301	778	526	469	284	327	299	495	376	352	301
306	438	273	470	399	411	184	441	461	545	610
615	572	619	297	620	115	970	601	999	662	557
682	972	955	243	928	188	934	221	281	658	658
295	841	830	787	345	424	216	506	271	488	583
402	344	251	673	636	330	274	203	311	393	556
330	373	273	292	322	254	218	333	278	270	251
278	285	439	494	455	442	464	459	451	447	381
446	516	341	693	682	368	648	463	641	641	638
356	273	341	613	599	607	218	358	240	366	361
379	364	354	393	282	278	329	443	459	304	363
418	466	173	208	295	340	675	229	271	367	130
301	466	472	245	399	357	354	409	436	261	285
384	203	415	474	288	416	309	319	390	201	467
232	711	148	262	314	20	332	249	512	294	202
397	0	426	237	335	253	350	356	623	638	24
317	118	344	398	303	656	253	397	549	794	482
358	377	276	279	416	207	361	116	532	293	509
184	492	598	452	539	285	198	404	269	202	593
292	602	674	330	220	341	640	360	610	153	696
364	920	169	903	256	429	866	243	861	353	640
573	658	246	681	300	319	266	363	236	672	594
471	225	330	797	858	667	317	506	556	329	357
201	360	523	502	578	507	320	433	508	482	640
410	397	509	512	478	480	478	553	265	471	400
475	451	236	517	521	151	583	188	605	588	590
258	407	315	396	290	368	270	397	314	343	

319

1884.8_2011EC37	272	281	140	346	310	288	326	246	627	252
250	364	278	356	417	394	269	442	416	361	393
465	266	491	286	251	446	325	358	497	429	460
487	466	488	545	838	178	740	384	357	285	384
240	315	674	353	186	358	350	245	255	298	614
337	684	699	700	286	348	692	334	803	307	439
330	800	480	445	271	443	279	464	332	363	306
404	463	256	480	313	485	213	448	501	661	772
785	675	781	229	774	163	641	646	662	999	654
993	638	649	184	680	198	655	257	273	885	885
319	635	645	761	377	518	256	453	356	462	568
499	208	284	702	669	538	300	251	371	452	633
375	378	253	350	328	176	202	356	265	269	240
336	206	417	514	433	416	430	477	421	470	466
485	630	518	650	664	494	622	592	732	620	735
502	233	317	646	597	615	206	414	181	433	425
388	368	403	436	224	276	418	434	587	265	355
454	407	177	253	272	326	657	240	175	366	141
256	411	534	246	503	343	401	424	463	370	266
293	202	258	326	335	384	330	336	402	217	539
189	792	191	313	318	117	242	252	605	358	191
462	0	490	273	364	319	370	319	609	760	212
243	157	404	509	324	710	204	487	617	819	600
340	323	227	280	423	227	369	182	691	333	730
166	531	668	443	614	295	237	421	251	179	668
303	718	629	304	173	231	790	437	744	155	630
313	544	173	571	242	446	718	186	730	390	793
656	711	215	596	356	285	189	336	285	589	686
467	179	366	608	597	673	390	537	634	317	293
210	313	602	517	650	601	296	431	688	452	563
476	380	711	584	581	513	495	723	411	532	479
625	490	210	441	655	181	594	226	630	631	680
380	536	358	394	371	385	285	420	335	338	

320

1886.0_1344EC16	284	278	169	305	306	295	314	234	635	209
277	299	297	388	425	460	314	332	388	358	335
441	251	479	301	241	411	321	291	525	393	517
514	502	391	457	751	166	632	421	303	271	287
319	339	504	287	211	386	282	225	298	250	450
325	668	672	669	279	268	664	299	663	259	432
282	684	459	442	243	271	268	458	358	349	265
334	425	260	389	357	435	203	385	426	971	680
690	975	687	363	698	148	555	537	557	654	999
654	535	554	127	576	168	567	205	248	602	601
310	523	534	636	323	382	218	429	268	435	426
371	270	261	534	512	358	226	211	285	391	516
295	325	242	278	255	296	115	321	274	289	169
242	258	379	476	399	382	406	438	399	432	334
445	483	425	535	542	396	517	467	662	535	659
403	122	291	517	474	484	207	386	257	431	399
413	349	413	451	147	319	335	432	427	141	330
355	442	136	214	267	314	642	244	193	317	156
293	437	464	253	356	383	300	388	460	246	294
268	194	232	331	301	353	268	321	406	140	467
204	712	162	278	322	28	301	283	496	302	186
419	0	523	333	304	240	337	312	665	671	247
271	189	330	451	271	636	224	396	593	696	484
354	342	276	310	397	272	385	171	609	267	579
150	550	538	501	452	275	255	350	225	208	571
201	574	496	288	229	336	737	317	722	188	518
317	471	146	513	237	429	604	183	626	358	612
532	569	208	524	311	250	302	311	260	490	517
405	242	311	500	520	560	379	458	583	303	290
243	310	613	536	509	527	258	355	531	404	595
387	404	528	524	519	466	462	551	293	491	378
496	371	248	459	499	100	481	219	490	501	489
276	421	274	329	294	369	260	363	290	308	

1886.5_2011EC38	280	296	188	347	312	291	320	246	625	236
252	357	275	369	401	394	254	446	415	357	404
471	268	490	287	267	448	334	364	501	430	468
489	472	489	546	838	229	743	388	358	290	380
253	321	676	358	187	379	354	257	277	298	616
334	709	713	718	279	351	709	327	802	299	434
328	801	476	440	253	435	282	458	333	363	308
405	467	256	491	338	499	215	433	502	662	771
771	675	764	234	752	176	660	648	682	993	654
999	660	670	210	702	206	678	259	288	887	888
316	635	645	759	372	535	255	453	358	462	576
516	208	282	703	670	541	287	250	382	460	630
344	388	254	351	324	186	227	374	267	273	248
330	212	435	512	452	435	449	496	440	471	467
485	630	524	665	679	490	637	590	733	632	725
507	264	318	651	609	625	219	416	167	434	426
396	370	404	437	265	278	411	434	596	306	356
464	409	162	227	276	320	655	242	146	362	139
267	411	541	269	505	351	403	424	469	375	290
307	228	259	329	335	387	343	349	402	285	538
188	794	191	312	320	107	263	235	620	357	184
461	2	487	271	371	322	367	339	608	795	154
273	165	405	516	342	707	187	484	609	819	600
333	351	199	296	429	236	370	215	691	345	732
174	523	668	443	615	297	242	439	265	184	671
290	715	620	309	186	240	788	438	721	170	636
308	551	171	576	257	426	718	210	731	385	792
651	713	213	601	350	313	197	353	290	595	681
472	179	366	606	597	655	390	521	620	333	303
214	334	588	513	654	589	309	455	672	477	565
478	381	716	584	587	514	500	721	405	533	479
626	489	242	469	651	175	594	228	642	642	680
386	562	354	403	390	386	277	430	329	355	

322

1889.8_1185EK16	296	313	199	318	307	282	331	230	656	273
274	315	310	376	423	495	326	327	396	366	347
421	258	494	274	272	436	350	290	646	362	632
660	668	407	475	681	265	622	342	351	305	324
316	316	533	307	199	333	340	193	264	291	453
330	604	622	617	279	286	606	285	724	276	469
290	752	527	469	276	321	297	492	380	335	299
303	432	262	469	398	411	179	426	452	524	572
578	553	585	277	586	137	982	589	972	638	535
660	999	965	228	899	143	935	221	267	639	639
283	813	802	757	326	430	188	500	255	482	575
389	339	227	659	622	325	269	203	304	388	549
311	366	251	261	282	255	205	309	263	287	212
278	270	434	479	447	438	457	450	440	443	358
438	506	312	687	671	353	641	451	633	635	623
339	242	340	599	594	602	206	332	193	330	338
324	311	319	339	262	198	322	369	454	272	337
421	451	150	211	274	331	673	247	278	347	131
306	435	468	234	385	344	317	401	423	264	283
398	205	412	489	268	428	299	303	403	208	474
209	693	149	265	316	24	306	235	525	271	194
394	0	407	213	324	240	328	328	609	620	28
301	117	342	394	291	641	263	388	536	768	469
348	379	247	238	406	196	361	109	510	293	498
186	491	573	449	529	289	198	402	256	209	586
231	587	679	342	217	290	586	359	576	95	693
244	923	157	909	241	428	839	224	834	335	631
567	644	235	703	308	302	273	360	229	699	571
465	224	324	780	846	654	311	498	542	309	358
211	345	491	478	560	482	310	429	486	473	621
407	396	493	509	472	499	464	540	278	462	390
461	431	244	519	516	157	586	184	599	583	583
257	402	302	392	278	366	253	392	315	351	



323

1894.9_1185EK17	285	328	187	310	273	275	299	216	681	249
232	327	310	367	382	481	289	309	410	377	370
404	242	484	257	249	429	353	285	660	359	663
668	682	387	441	711	227	637	333	316	290	311
301	274	545	320	210	325	332	190	256	268	436
327	630	636	633	248	285	624	255	748	272	462
264	785	514	456	263	336	301	487	369	333	271
292	448	241	449	382	381	171	394	444	530	587
591	583	604	255	601	134	969	621	955	649	554
670	965	999	169	929	160	982	199	247	642	640
267	823	812	768	319	427	193	501	241	481	536
373	331	196	637	605	323	266	192	284	367	537
292	375	227	234	266	253	161	326	251	259	223
276	261	431	466	443	419	448	459	450	424	361
406	493	346	673	663	357	628	452	645	637	630
358	224	328	599	586	602	198	304	208	303	311
293	314	292	310	235	162	312	323	458	241	331
438	464	192	194	268	299	699	237	269	342	126
325	436	489	228	385	345	326	413	416	263	270
374	198	424	476	253	374	281	286	405	218	477
130	715	174	254	300	16	305	240	514	292	176
405	0	393	175	304	245	314	296	637	650	32
293	101	337	408	301	683	261	384	533	800	481
356	388	326	244	382	167	360	112	494	285	519
187	486	580	429	532	291	162	397	264	201	572
243	605	707	339	193	261	608	378	598	70	701
260	920	160	918	236	440	849	195	849	331	644
593	637	186	707	302	272	256	350	234	697	531
454	332	319	798	861	666	369	512	567	296	315
209	339	487	479	569	478	311	430	482	466	624
420	399	509	477	452	505	494	547	317	512	394
468	423	216	487	515	130	593	209	584	607	596
254	426	299	387	281	351	259	386	300	326	

1900.0_1135EC04	179	232	700	171	174	119	185	195	155	173
315	111	180	170	194	159	159	247	271	275	109
150	235	125	164	302	153	200	118	167	203	62
196	134	245	156	82	801	351	140	199	235	305
254	187	164	187	135	263	237	174	241	195	183
194	224	203	206	189	139	214	233	32	206	228
259	107	242	247	212	267	208	251	319	254	247
243	285	234	237	209	343	211	216	304	204	129
160	115	149	3	126	294	242	211	243	184	127
210	228	169	999	299	175	260	369	214	263	256
112	111	70	101	232	233	177	283	230	269	316
244	173	207	91	95	125	199	174	199	235	193
213	199	279	207	202	223	935	246	450	103	267
224	197	275	242	318	297	259	309	230	269	305
277	159	186	209	193	271	210	152	205	225	213
290	891	129	203	200	194	259	181	52	246	204
149	3	161	0	869	169	279	251	211	874	163
106	220	293	240	167	185	117	146	172	59	235
168	0	258	278	212	170	0	0	120	0	176
94	179	117	92	173	271	306	175	179	156	71
126	75	200	59	86	192	243	68	96	109	14
140	129	123	183	216	218	191	163	65	208	47
187	125	151	179	77	154	167	218	180	44	299
110	20	6	432	115	199	164	126	69	235	0
148	244	23	0	139	2	188	52	205	192	225
240	142	158	172	212	174	49	25	108	141	144
0	202	140	50	202	92	86	226	65	66	203
57	179	156	81	204	277	210	252	173	110	116
91	1	49	305	86	117	108	32	154	267	300
151	263	242	91	96	246	134	76	128	107	2
11	131	310	62	279	66	261	80	19	215	199
43	199	5	118	205	5	203	147	108	58	40
256	61	309	356	198	160	162	174	139	161	

325

1906.6_1185EK19	291	332	259	321	289	293	289	229	697	238
230	341	302	369	398	453	276	339	426	375	378
434	230	497	261	260	450	343	300	649	390	650
656	665	403	450	725	313	673	334	326	290	299
245	302	539	315	206	342	334	197	276	292	462
348	651	668	664	246	305	651	258	761	270	466
264	813	510	467	267	347	281	494	377	354	284
308	449	235	430	403	416	182	398	451	547	613
618	598	637	257	628	144	905	615	928	680	576
702	899	929	299	999	189	958	205	262	677	676
262	808	795	765	346	421	226	510	272	493	602
373	267	237	658	619	334	271	185	294	375	546
320	373	242	271	311	261	297	351	274	260	257
288	257	412	477	430	403	443	461	443	431	378
411	517	363	679	665	380	629	460	658	640	642
385	368	331	617	589	604	225	315	212	318	335
294	323	310	323	361	226	344	371	466	350	335
431	457	222	201	278	289	714	257	258	330	120
310	436	530	264	402	334	324	411	449	263	294
356	190	412	457	280	368	290	299	407	181	475
129	730	175	261	306	15	247	233	501	282	177
424	0	410	186	309	258	336	288	652	672	33
314	122	356	416	284	694	240	403	558	820	495
365	389	296	299	388	187	358	137	518	311	535
170	505	604	441	534	289	185	400	270	215	598
256	616	695	336	219	226	637	379	629	120	709
268	874	141	866	257	415	829	214	833	346	654
595	664	204	645	304	323	276	372	246	628	576
457	335	333	787	827	672	390	540	586	342	367
196	363	507	493	585	493	297	408	504	463	632
415	350	552	489	483	506	513	557	321	554	401
469	425	220	488	525	149	596	221	591	603	597
263	414	313	417	306	363	272	391	303	341	

1908.3_1344EC04	197	230	160	262	233	133	216	265	218	217
280	181	150	186	194	164	190	196	223	247	143
230	176	223	172	193	172	172	202	138	227	118
142	127	152	185	162	232	196	145	176	220	269
203	192	150	185	110	222	199	306	189	170	179
351	188	154	133	201	203	166	252	152	225	167
225	179	219	167	230	297	181	201	266	276	225
280	245	271	188	225	285	352	140	228	241	112
180	125	125	156	102	351	156	177	188	198	168
206	143	160	175	189	999	202	252	197	205	214
223	153	149	154	270	169	153	228	245	227	124
175	154	239	198	165	184	239	206	313	235	208
272	258	177	255	168	188	217	109	246	98	167
254	164	260	273	256	255	254	266	222	263	291
283	165	197	165	171	357	182	213	200	223	203
248	222	164	196	191	179	276	161	105	204	217
184	44	189	116	195	142	346	185	234	209	187
197	169	269	156	135	216	189	287	209	196	245
150	138	141	147	202	120	110	235	221	166	178
150	160	176	203	168	231	208	137	131	168	157
61	179	79	129	146	166	131	182	147	132	111
195	168	189	194	193	119	334	157	118	127	12
232	203	190	250	161	160	187	200	189	120	255
119	138	150	197	132	224	258	171	200	198	135
114	223	82	160	238	221	216	189	229	72	207
171	163	157	203	211	141	97	129	82	272	141
139	95	186	99	172	180	117	191	146	202	168
145	164	185	142	176	315	197	225	176	121	193
189	4	165	175	104	134	205	221	207	301	257
198	218	199	172	123	181	123	139	146	196	193
150	239	210	183	206	150	270	187	161	178	196
151	230	78	99	215	136	94	229	154	120	194
221	106	293	279	298	315	296	346	322	188	

1908.5_1185EK16	291	324	219	331	305	287	318	217	690	237
244	308	307	371	416	491	302	316	430	372	365
405	237	491	261	266	460	345	291	662	364	664
666	681	398	446	713	267	646	337	335	303	316
270	301	554	324	237	350	331	215	279	283	444
348	640	643	642	264	293	633	258	751	286	458
284	796	511	453	275	338	286	485	374	345	272
291	445	238	430	400	390	191	409	448	537	612
621	593	620	261	627	141	940	606	934	655	567
678	935	982	260	958	202	999	196	258	654	654
281	783	773	746	322	431	194	523	249	503	574
375	273	210	648	609	332	295	189	314	373	555
304	376	235	244	275	254	256	327	269	280	238
300	264	424	472	441	412	449	464	452	425	364
410	500	359	671	657	386	623	438	647	636	630
373	340	335	596	582	597	210	324	176	325	333
314	333	314	332	335	205	346	337	444	325	353
434	471	147	197	279	318	708	237	252	333	127
324	448	522	254	391	344	320	414	414	269	299
387	205	422	473	255	401	283	299	414	181	482
170	721	177	256	298	140	280	235	508	303	211
413	0	416	212	310	246	336	298	642	660	29
311	121	343	411	264	678	261	391	555	806	484
362	384	306	293	381	185	364	141	508	304	528
171	488	610	423	528	289	183	406	274	204	583
229	607	708	322	214	301	618	367	602	155	704
266	881	176	885	254	434	814	224	815	329	642
597	644	199	676	313	302	278	366	237	665	580
454	239	324	766	826	682	347	526	582	317	351
210	360	512	494	569	498	310	425	489	470	646
411	360	518	499	479	511	507	531	309	532	404
455	419	182	499	502	128	599	241	579	601	586
261	406	317	409	302	373	290	392	318	327	

328

1914.2_2011EC35	291	323	236	308	308	329	299	218	241	236
197	298	753	287	181	226	286	180	163	353	327
344	187	282	571	244	229	592	353	275	323	243
279	262	198	210	258	285	313	395	317	329	197
204	658	301	265	217	232	276	251	337	712	252
289	249	237	243	247	274	241	303	231	269	207
311	231	246	211	288	228	689	224	143	193	223
209	191	462	217	225	249	209	258	173	223	203
195	200	218	177	213	243	218	245	221	257	205
259	221	199	369	205	252	196	999	497	253	251
259	214	215	234	299	232	204	204	309	203	262
207	175	146	238	259	230	327	899	295	352	241
325	322	200	191	224	463	338	258	261	217	201
330	481	219	214	230	245	204	213	237	294	227
183	167	139	239	229	235	231	187	228	221	246
191	330	232	217	233	219	231	160	222	158	207
171	251	170	199	371	205	336	170	228	341	288
292	207	230	818	334	299	255	235	210	312	147
702	174	258	256	199	269	202	287	322	306	326
257	570	321	369	299	181	373	391	215	107	263
201	261	181	245	314	203	206	464	269	297	201
210	309	221	159	271	292	299	276	229	240	25
216	213	288	238	279	236	280	288	266	231	274
273	142	322	292	253	603	204	444	178	264	242
670	266	241	247	243	182	448	196	313	138	293
169	217	272	246	616	109	211	242	215	235	282
119	166	297	180	494	274	212	183	212	306	253
217	249	679	242	155	275	401	272	740	262	210
278	169	743	261	197	302	599	440	367	273	299
213	254	328	235	238	188	235	232	203	211	265
240	196	232	227	204	249	357	214	266	250	206
213	247	149	233	233	263	268	255	242	230	212
221	236	298	323	286	301	331	334	335	245	

329

1916.6_1164EK04	355	336	201	413	386	309	356	177	311	302
301	322	537	460	293	312	344	254	273	340	384
389	228	355	499	309	287	464	400	314	459	284
315	300	278	273	274	172	337	407	343	412	418
549	548	377	308	195	433	505	282	326	633	308
342	257	262	256	393	345	255	290	255	255	243
292	267	247	243	309	249	556	228	263	205	525
238	230	538	265	238	316	199	368	257	288	229
241	252	253	343	256	197	292	315	281	273	248
288	267	247	214	262	197	258	497	999	289	287
206	252	254	253	342	244	274	293	266	290	228
214	300	168	269	252	229	238	499	262	362	266
274	337	271	231	412	566	190	375	335	289	198
258	587	235	243	256	268	243	279	280	295	278
212	209	264	270	268	226	271	242	252	264	257
237	161	190	258	286	268	214	201	145	186	219
210	211	189	154	196	213	294	231	229	181	387
339	285	147	535	312	356	342	149	291	359	158
540	251	285	255	253	335	313	322	399	253	357
299	572	332	380	425	285	484	429	260	161	279
361	318	251	394	425	282	548	543	346	364	190
262	0	289	281	417	516	318	403	298	282	195
336	108	394	281	302	310	382	381	304	285	294
214	280	328	349	259	577	249	399	230	524	241
463	318	258	185	283	243	493	273	286	278	425
202	287	298	219	725	181	282	220	254	143	302
280	236	138	260	948	232	249	219	256	360	318
286	258	621	299	207	257	439	255	536	324	261
258	58	553	305	275	412	451	465	433	278	299
236	241	408	237	295	217	232	244	215	221	350
263	206	281	389	411	288	357	278	228	275	298
276	257	71	251	271	182	285	120	299	294	277
268	220	298	302	282	298	241	309	302	272	

330

1920.6_2011EC41	298	301	199	326	321	315	307	248	603	231
275	391	293	367	416	426	253	442	436	385	424
462	257	510	287	263	507	350	341	502	429	478
496	487	507	550	787	245	715	398	387	302	386
250	345	637	362	219	373	368	285	296	313	617
328	641	652	688	298	379	648	320	768	281	468
306	786	472	474	252	461	273	489	376	379	325
369	536	255	474	371	496	225	411	515	619	716
693	632	682	252	696	160	643	669	658	885	602
887	639	642	263	677	205	654	253	289	999	994
355	648	662	730	348	585	257	521	359	523	640
619	295	293	690	703	593	293	232	375	463	660
354	382	240	355	328	195	278	342	304	296	274
336	210	436	457	452	438	441	496	447	466	496
492	596	505	672	683	516	649	582	712	655	689
494	312	315	664	605	627	223	451	228	447	464
429	440	434	457	304	320	421	483	580	340	348
475	405	173	209	288	307	641	238	125	390	165
267	430	564	271	493	353	419	466	474	377	282
309	193	275	359	321	407	360	334	423	261	569
213	776	231	294	360	96	260	253	590	363	230
468	2	471	278	388	340	369	351	638	701	136
268	177	415	505	341	716	186	464	598	812	622
329	322	198	306	431	244	386	189	628	331	711
179	538	662	421	633	276	263	402	293	211	655
317	731	636	313	195	273	737	479	679	145	628
370	574	160	602	270	493	705	204	718	369	788
684	774	222	649	387	331	240	367	294	640	717
447	163	359	646	612	635	361	518	628	354	309
247	352	585	553	687	571	301	455	627	453	560
515	445	686	553	562	493	521	699	398	525	491
622	477	199	524	666	162	602	262	649	659	687
391	532	377	432	406	406	314	453	355	342	



331

1921.2_2011EC40	294	299	184	324	319	312	307	249	602	232
273	385	289	369	410	425	254	445	436	373	406
464	260	508	294	269	501	347	344	495	429	472
487	480	516	549	787	226	711	397	362	302	389
252	344	642	365	215	377	364	299	303	300	620
326	643	654	690	300	371	649	320	770	279	456
307	788	458	461	251	456	271	476	375	379	329
367	538	248	480	390	507	253	417	500	620	719
694	632	686	255	699	176	642	669	658	885	601
888	639	640	256	676	214	654	251	287	994	999
360	630	646	731	346	586	252	524	368	525	644
620	279	296	697	710	601	301	230	375	461	668
360	388	235	356	331	214	267	347	293	292	270
342	217	437	459	453	440	442	498	449	459	495
493	598	506	672	683	508	648	585	698	653	678
498	288	312	666	606	629	221	434	224	435	449
425	461	424	454	290	320	434	483	581	317	349
471	395	173	207	291	307	641	241	125	383	167
265	426	568	237	511	345	420	458	472	376	271
306	217	286	351	322	404	354	329	434	227	564
183	775	232	271	329	97	262	247	568	369	227
468	2	470	279	380	333	367	346	638	702	159
275	176	411	507	341	718	213	463	595	812	620
328	322	196	323	435	255	387	203	632	334	715
177	540	653	420	631	272	255	420	286	200	658
302	731	643	310	198	266	740	481	682	165	627
369	557	175	586	268	493	704	180	718	367	785
685	776	228	647	384	328	247	364	293	637	725
446	163	356	628	594	634	360	512	624	351	312
248	344	585	546	689	571	302	456	628	454	560
515	444	694	543	543	496	513	677	398	524	488
619	480	189	524	665	173	602	266	649	660	688
394	526	377	429	414	410	322	467	375	345	

332

1924.7_1164EK03	227	232	0	248	235	254	208	220	365	128
215	269	213	294	229	262	157	226	228	289	244
321	223	411	234	272	268	301	235	347	308	319
348	327	310	378	361	0	334	235	232	279	182
265	253	337	235	213	320	276	252	270	237	366
303	303	302	292	250	202	282	316	342	257	313
303	347	339	321	243	305	238	330	258	290	268
259	243	217	269	516	415	283	197	270	332	291
285	314	289	195	294	230	313	328	295	319	310
316	283	267	112	262	223	281	259	206	355	360
999	293	309	328	301	304	236	270	635	283	302
289	279	394	341	339	307	544	255	316	292	276
870	302	196	446	226	165	100	281	292	298	146
564	174	273	315	333	302	267	372	402	442	316
264	271	298	327	325	335	311	295	322	379	334
366	0	223	308	343	349	292	313	229	423	340
340	245	355	337	54	298	319	404	303	0	249
262	275	177	213	203	208	392	225	126	245	164
221	258	305	218	278	247	228	316	375	292	163
275	160	241	323	277	289	199	191	302	250	372
151	343	160	183	247	115	257	225	316	240	218
282	301	309	165	239	232	302	209	309	323	240
260	183	224	319	256	331	157	278	348	357	350
192	301	190	227	224	217	318	108	273	285	323
168	317	287	217	326	249	167	266	212	0	320
219	319	309	235	210	167	290	235	297	225	304
285	235	230	312	209	286	312	233	335	305	316
293	339	203	298	235	262	151	231	279	281	295
264	75	242	316	272	320	148	269	305	261	233
308	231	257	280	347	271	303	249	249	253	271
233	240	274	346	273	333	378	306	133	286	242
295	261	175	304	337	135	309	169	329	331	310
227	236	299	288	324	340	284	362	310	218	

333

1927.7_1288EC32	257	232	118	315	311	243	325	234	598	211
256	300	259	294	367	387	273	284	327	337	343
390	216	429	238	263	387	272	308	514	357	510
501	505	384	483	705	165	619	282	320	255	310
278	295	571	305	179	307	269	199	264	254	457
301	617	650	654	253	277	615	292	750	259	418
301	787	473	424	260	290	236	461	359	329	263
339	412	228	497	341	428	188	418	451	550	667
653	545	634	278	615	111	812	561	841	635	523
635	813	823	111	808	153	783	214	252	648	630
293	999	979	852	307	399	211	513	292	520	644
412	307	260	754	705	377	258	221	274	361	554
316	304	273	284	243	158	101	275	280	224	220
274	153	435	471	456	438	453	471	440	471	431
474	551	359	658	673	382	640	516	684	654	673
403	155	316	636	571	590	219	392	275	427	394
385	399	422	434	151	268	311	408	506	142	315
328	407	101	200	233	325	621	216	167	291	105
283	387	483	253	321	329	354	356	378	305	213
247	148	223	319	256	349	212	229	327	217	474
205	658	87	216	281	41	272	206	511	289	203
400	0	430	256	273	259	303	284	570	649	31
242	167	316	367	279	655	202	384	540	794	490
320	343	327	230	434	188	331	64	551	269	577
147	495	643	423	534	255	174	319	177	216	564
293	626	682	286	179	297	689	346	677	120	672
412	798	125	817	207	374	966	201	943	337	589
572	706	191	663	224	238	191	318	224	662	578
397	195	298	857	893	745	405	525	601	271	232
165	323	535	550	574	513	294	437	487	457	529
409	395	480	540	506	516	422	548	270	455	436
513	399	195	502	591	189	532	126	568	562	565
293	413	264	316	276	308	251	334	235	270	

334

1931.1_1288EC35	258	234	64	316	312	244	325	237	603	211
254	300	260	300	366	387	274	286	310	342	344
386	214	433	239	269	383	271	307	512	361	511
498	503	391	489	713	78	622	284	334	258	313
280	292	558	306	178	308	270	197	262	254	453
303	631	667	670	254	286	632	297	767	260	420
305	801	477	428	264	297	236	466	359	333	261
344	413	227	490	340	432	189	414	455	561	682
667	555	647	278	627	111	801	567	830	645	534
645	802	812	70	795	149	773	215	254	662	646
309	979	999	872	310	406	213	514	291	521	632
413	306	263	764	709	370	259	221	278	367	563
315	312	279	288	244	156	64	275	280	225	209
274	152	439	478	462	440	457	477	444	462	435
479	564	367	664	679	388	644	528	698	657	686
415	96	306	653	585	603	221	398	279	440	402
376	411	434	445	91	263	312	420	519	86	316
329	410	106	200	234	325	626	219	166	292	102
283	386	483	237	327	331	356	359	372	288	215
247	148	223	322	256	353	218	223	339	217	480
205	664	87	219	300	47	272	204	498	289	203
404	0	434	256	274	257	305	285	572	660	13
235	170	327	369	278	669	199	394	549	808	497
300	343	326	221	451	188	331	68	563	267	573
147	493	646	427	547	255	173	331	161	219	572
293	631	682	285	180	309	706	350	695	104	670
399	787	129	807	206	377	965	202	955	336	598
577	706	193	663	227	234	182	308	225	661	586
396	196	299	841	877	747	411	529	603	268	229
166	316	541	548	580	521	302	439	495	461	530
412	399	492	552	519	520	420	561	275	450	436
528	403	195	514	604	181	537	129	585	575	584
299	423	268	310	277	309	253	335	236	274	

335

1935.5_1288EC36	270	236	55	332	325	255	333	249	616	231
261	305	269	303	359	370	285	317	342	352	360
431	229	464	243	281	373	284	331	491	410	483
479	481	406	501	788	103	690	308	361	276	333
281	297	568	331	180	322	289	211	282	258	478
326	746	757	756	296	306	752	328	874	273	443
336	881	476	459	277	350	249	456	359	379	271
377	420	230	460	351	456	205	397	467	649	804
788	658	807	299	784	113	758	592	787	761	636
759	757	768	101	765	154	746	234	253	730	731
328	852	872	999	346	433	217	506	341	513	581
438	289	292	737	688	421	277	217	308	380	636
332	335	294	325	287	144	94	312	278	262	196
289	155	449	553	461	441	471	485	448	453	436
502	617	403	649	663	427	638	551	764	643	746
456	121	299	691	602	616	225	441	291	520	450
427	472	511	533	113	312	318	505	526	119	329
330	387	126	191	243	333	633	242	170	300	94
280	372	471	235	319	333	376	370	417	274	221
248	142	227	331	306	331	238	252	318	260	505
236	715	87	219	307	56	271	218	545	316	216
420	0	464	238	287	230	341	297	594	774	37
221	185	365	378	259	742	183	419	597	893	529
303	359	314	238	461	185	348	71	660	263	621
141	532	692	430	591	259	192	359	177	214	631
298	653	651	284	181	293	819	396	815	149	642
398	672	117	705	234	374	899	221	911	369	662
602	698	187	689	301	229	178	305	234	669	640
437	219	325	743	758	744	462	539	654	267	230
181	301	652	539	608	587	323	448	607	480	555
425	393	595	604	561	518	407	628	299	483	462
549	458	205	481	610	183	547	142	620	605	629
317	462	254	315	277	295	254	325	236	280	

336

1939.9_1185EK11	321	328	230	476	365	328	375	263	426	369
202	377	352	431	260	290	341	260	314	363	528
582	201	393	396	234	288	387	709	308	658	321
320	318	298	337	377	263	349	373	498	366	181
255	343	402	680	249	300	334	287	267	323	303
770	337	353	353	335	350	350	215	363	256	285
228	370	319	291	241	335	320	310	284	304	322
255	280	305	217	338	275	239	226	276	328	344
357	321	353	287	344	261	323	314	345	377	323
372	326	319	232	346	270	322	299	342	348	346
301	307	310	346	999	276	225	263	359	260	274
244	214	202	313	319	242	321	278	325	329	270
364	292	196	295	330	243	218	538	272	316	187
329	277	266	257	280	268	230	271	259	335	229
252	291	234	311	310	303	326	288	332	307	323
301	215	235	289	326	322	206	242	73	249	253
245	232	231	253	232	200	318	229	253	206	467
400	346	312	332	345	375	443	289	321	408	103
333	218	324	256	272	333	452	339	612	265	252
301	243	333	388	595	298	304	435	345	146	342
219	342	218	190	496	156	234	224	314	667	234
227	356	252	203	371	319	737	299	302	367	83
258	135	396	330	299	370	224	385	325	365	329
211	250	271	269	290	320	269	178	397	305	294
210	340	342	294	297	317	326	275	326	96	413
202	290	343	255	275	204	346	282	336	269	278
148	250	386	273	322	339	309	292	330	944	363
273	345	306	330	333	286	270	272	334	345	271
357	139	300	329	279	330	267	301	338	299	322
255	258	361	332	308	293	227	253	320	190	287
209	240	318	299	274	261	381	307	249	300	244
260	261	95	276	301	158	337	223	305	323	263
190	241	274	286	307	322	307	323	303	254	

337

1940.3_1288EC07	256	272	225	275	282	259	340	238	373	283
276	312	304	336	326	351	301	357	339	318	292
367	289	354	275	292	354	298	300	413	317	391
423	407	326	386	486	281	458	309	325	305	250
225	310	429	229	174	252	250	200	303	275	492
274	470	490	484	258	305	479	306	473	322	437
315	476	475	427	322	265	244	443	272	308	242
270	343	273	412	317	401	170	301	380	372	438
443	363	467	322	453	140	434	464	424	518	382
535	430	427	233	421	169	431	232	244	585	586
304	399	406	433	276	999	242	415	295	415	571
899	244	261	480	614	777	263	188	274	366	466
344	317	224	305	344	237	221	347	229	172	209
274	234	323	391	337	374	338	359	380	438	411
327	418	304	502	500	390	460	443	468	477	469
346	239	230	417	490	497	172	353	246	316	389
358	315	315	328	197	298	326	386	428	251	273
449	351	179	272	248	340	391	229	232	307	155
296	354	450	253	400	361	299	395	372	343	245
423	250	418	418	275	312	273	324	334	183	415
214	507	145	243	312	32	230	269	407	239	151
412	0	374	232	318	243	294	282	420	510	23
289	128	339	345	295	437	233	287	381	473	423
268	358	223	246	341	234	382	154	403	285	469
196	396	376	267	451	254	216	314	205	218	446
233	500	437	208	213	222	459	329	433	170	400
410	407	145	415	225	423	431	229	442	283	510
465	534	219	440	268	255	248	261	301	419	484
353	75	304	413	360	360	267	342	380	246	276
189	242	395	300	460	386	281	344	444	352	430
340	312	387	332	318	343	373	463	243	397	333
434	356	198	429	461	152	446	164	487	480	432
213	374	298	351	284	333	201	350	302	249	

338

1940.4_1344EC27	295	328	123	281	292	291	318	92	284	187
186	291	222	283	157	232	269	170	149	316	207
289	256	278	254	207	299	297	232	309	310	289
320	295	291	252	256	107	244	334	340	303	168
227	218	281	183	306	319	303	223	305	240	227
235	210	223	220	221	303	211	213	260	259	255
227	236	230	251	223	199	182	227	207	180	314
218	212	242	211	208	243	207	219	165	244	182
171	228	181	281	185	166	240	271	216	256	218
255	188	193	177	226	153	194	204	274	257	252
236	211	213	217	225	242	999	182	230	182	197
215	318	189	190	208	219	237	199	122	286	172
289	345	224	215	368	318	173	246	338	291	185
230	364	238	204	232	228	251	297	261	234	178
224	180	154	252	254	190	247	200	240	236	223
234	91	227	242	278	284	226	158	37	184	141
147	35	140	150	129	154	262	195	221	85	268
255	121	117	172	266	318	274	108	223	346	86
151	172	251	77	184	221	212	241	311	209	470
232	228	376	364	307	233	285	319	267	127	222
389	193	197	325	331	202	195	257	254	185	277
142	0	165	175	278	272	204	201	263	225	161
309	0	326	209	243	245	244	291	220	267	279
209	207	102	298	166	321	211	134	213	297	146
216	187	248	149	235	169	234	144	167	218	292
103	207	362	250	249	2	212	200	201	111	321
11	208	228	211	267	185	201	54	210	220	284
232	194	287	277	226	254	236	268	220	290	147
176	5	153	245	251	247	169	234	266	241	282
211	264	257	183	296	191	250	152	169	215	259
215	215	200	272	260	244	327	248	75	216	175
226	255	218	216	257	220	242	66	256	267	231
164	184	265	268	272	233	251	246	231	267	



339

1946.4_1164EK02	302	299	159	257	270	306	270	270	683	221
297	351	330	398	536	483	241	363	503	308	327
328	244	460	283	303	437	322	235	635	275	610
652	648	427	515	556	219	550	320	290	245	289
268	360	513	275	220	324	248	231	260	276	409
262	420	429	432	248	277	421	327	502	304	438
300	516	491	447	277	370	264	479	449	344	271
321	403	292	390	367	453	208	386	382	439	419
426	443	448	306	473	140	529	485	506	453	429
453	500	501	283	510	228	523	204	293	521	524
270	513	514	506	263	415	182	999	295	993	495
441	186	152	496	494	367	276	219	310	400	417
319	356	233	221	221	233	249	262	196	189	312
288	212	326	359	329	305	322	337	323	421	324
360	395	328	486	485	357	484	401	520	486	535
342	296	315	463	439	455	247	310	258	350	308
307	292	324	318	331	206	402	330	405	313	266
430	388	181	177	279	270	661	288	167	391	209
342	435	474	340	447	343	275	509	394	315	296
327	231	281	386	192	446	346	295	443	167	496
188	575	233	277	278	69	272	227	465	273	179
472	0	414	281	338	210	253	270	505	449	80
289	170	315	549	317	513	191	380	546	526	477
398	340	298	303	400	265	363	203	370	295	440
214	499	465	366	399	332	258	397	264	229	476
379	456	473	345	238	332	430	289	411	168	465
214	488	196	503	262	531	540	225	546	282	536
433	543	270	429	414	307	230	365	274	428	462
328	190	289	511	494	497	176	432	445	330	303
187	359	387	433	411	409	265	286	320	319	495
326	314	440	408	412	360	498	475	279	472	357
390	351	167	469	451	175	396	245	426	432	445
323	403	357	380	381	409	358	441	364	301	

340

1947.0_2011EC48	219	285	143	285	298	274	260	247	322	156
270	298	263	268	251	248	230	228	169	307	264
331	255	362	227	226	288	274	302	269	317	285
261	265	270	338	376	169	354	246	289	332	278
227	267	338	263	226	302	262	284	296	245	401
318	319	301	304	331	211	298	289	345	252	306
270	338	309	315	251	331	259	311	260	302	261
259	274	270	258	632	364	268	233	282	326	301
303	269	324	149	297	230	268	336	271	356	268
358	255	241	230	272	245	249	309	266	359	368
635	292	291	341	359	295	230	295	999	293	281
299	309	556	356	346	308	369	286	342	292	269
660	301	247	605	299	204	228	257	295	310	209
395	199	257	302	274	278	254	320	322	382	305
265	248	216	286	292	327	280	259	351	309	328
312	199	184	282	280	288	324	414	197	517	434
443	282	490	427	209	414	371	550	300	233	266
274	239	245	191	285	260	324	240	124	344	137
238	201	281	192	221	244	239	292	360	179	229
228	193	250	260	233	254	263	281	215	143	316
257	307	166	156	269	218	219	220	283	265	216
211	262	234	223	291	211	304	247	258	297	34
282	145	238	169	239	319	194	253	258	343	338
223	183	162	256	201	244	243	165	267	268	249
155	287	285	213	296	223	238	262	290	183	327
214	291	280	215	241	233	313	273	282	228	325
221	188	291	227	273	247	315	192	314	331	331
308	324	285	323	235	261	197	247	232	284	256
210	121	200	307	227	237	157	196	253	284	250
261	246	252	289	309	252	258	187	244	242	213
212	240	279	289	244	260	343	274	200	255	230
241	289	201	227	282	142	247	245	269	251	275
231	206	344	353	321	383	348	397	375	260	

341

1957.4_1164EK02	303	298	161	255	269	303	275	268	681	246
	296	347	329	399	537	488	260	363	486	293
	326	246	459	280	293	449	314	232	634	269
	653	650	424	518	563	225	547	315	290	236
	263	364	518	272	221	322	243	228	267	276
	260	422	427	431	247	274	424	322	509	314
	298	522	484	441	291	365	265	472	448	347
	325	404	290	393	368	450	207	385	382	444
	432	444	455	308	480	127	511	490	488	462
	462	482	481	269	493	227	503	203	290	523
	283	520	521	513	260	415	182	993	293	999
	432	186	155	503	496	371	277	218	312	379
	330	359	229	224	226	231	243	269	193	189
	286	218	314	367	318	294	313	330	312	421
	360	406	332	489	490	364	487	409	526	491
	345	288	311	472	445	461	252	310	257	348
	307	291	324	318	323	207	406	326	413	306
	429	390	178	177	275	275	658	288	200	387
	321	439	474	352	450	341	275	508	393	327
	323	230	285	384	183	448	338	292	442	167
	186	584	225	273	278	69	267	224	463	270
	468	0	420	275	339	204	251	272	507	447
	314	170	313	547	317	513	225	410	556	530
	395	361	302	305	411	263	366	217	377	292
	207	510	476	379	402	337	264	397	258	228
	377	464	490	342	236	349	438	286	418	143
	214	492	164	501	257	528	548	222	553	277
	438	544	270	433	409	306	233	361	273	433
	351	191	291	515	500	494	175	446	451	326
	182	355	389	429	408	413	264	272	333	307
	327	315	429	406	413	359	495	477	293	477
	399	359	178	451	454	145	409	247	436	440
	314	412	366	383	372	417	358	445	378	300

342

1959.2_2011EC40	260	271	289	277	287	228	267	239	498	229
312	307	277	327	446	455	260	396	392	349	277
382	261	428	223	226	402	314	262	410	334	433
420	428	376	442	518	323	567	294	301	266	321
315	331	613	274	187	376	316	159	244	252	588
268	499	480	484	264	277	480	300	554	218	402
268	556	409	400	231	320	273	388	382	301	276
294	360	248	447	353	462	175	394	435	466	453
478	420	460	269	490	125	579	500	583	568	426
576	575	536	316	602	124	574	262	228	640	644
302	644	632	581	274	571	197	495	281	498	999
647	298	238	792	839	660	227	223	271	371	509
291	307	301	281	285	166	313	279	314	226	201
268	189	360	393	370	363	365	440	399	467	452
375	457	349	562	564	399	511	465	521	531	539
376	335	249	516	499	504	257	390	155	381	402
406	356	379	379	344	304	320	378	483	317	287
437	391	182	178	213	267	522	198	155	306	219
258	375	633	249	421	328	286	382	375	412	169
303	94	287	328	246	389	271	219	341	197	402
185	562	60	247	272	16	300	230	575	261	155
404	0	415	252	266	230	276	286	475	488	24
177	141	293	334	215	510	131	317	427	611	374
318	388	252	314	290	193	324	94	437	260	634
97	423	548	357	436	273	169	331	194	153	472
287	492	490	235	176	253	502	286	469	62	540
18	604	162	632	208	443	641	218	655	284	529
444	807	172	540	313	254	190	246	268	534	541
312	136	342	697	619	554	230	429	439	267	259
210	240	437	481	495	421	286	312	470	357	490
331	365	466	430	434	393	375	498	273	510	422
417	354	183	398	513	125	452	102	486	486	495
275	400	283	365	255	279	170	294	220	268	

343

1961.3_1288EC07	237	257	239	233	247	261	277	231	409	213
228	301	272	318	340	363	230	372	344	286	250
348	250	351	227	261	339	307	257	414	316	400
425	408	310	430	492	290	487	295	267	275	258
195	293	492	211	182	267	252	208	245	232	576
239	449	539	522	230	271	521	287	466	281	404
299	435	417	406	278	273	226	402	268	288	228
288	323	245	377	300	392	160	306	397	394	451
454	396	413	232	457	185	413	447	402	499	371
516	389	373	244	373	175	375	207	214	619	620
289	412	413	438	244	899	215	441	299	432	647
999	241	233	566	709	873	242	194	208	355	460
299	326	179	279	288	218	248	306	204	172	194
254	235	297	360	296	343	311	348	372	433	385
307	406	312	469	460	379	426	436	466	447	466
317	274	250	397	468	461	174	282	220	285	329
292	291	292	296	221	284	332	341	426	244	245
445	366	167	239	249	277	428	234	183	282	144
284	369	518	248	427	315	246	381	376	425	227
384	235	360	397	269	292	254	263	348	185	450
158	513	151	222	264	28	219	214	471	220	121
356	0	333	212	274	231	248	253	430	480	16
288	137	306	358	232	429	252	302	421	493	407
306	306	203	236	328	202	365	201	404	296	579
176	390	404	272	427	250	206	283	216	207	448
234	481	439	230	189	256	483	325	466	159	407
398	438	115	460	221	437	420	230	455	274	502
450	606	208	431	267	243	253	262	288	409	470
341	72	295	432	413	367	259	362	388	233	303
192	250	371	311	438	356	261	301	418	297	442
344	341	410	337	337	347	385	452	267	413	353
420	335	204	412	452	126	431	131	464	450	412
210	364	307	366	303	344	209	362	313	259	

344

1975.9_1344EC27	237	283	141	290	280	228	225	170	243	208
180	263	203	296	208	260	183	251	233	246	198
327	269	299	252	242	294	235	251	265	358	262
286	267	239	237	232	136	245	293	262	347	236
255	313	249	196	220	353	275	235	255	266	247
217	188	224	210	328	290	212	249	260	195	263
225	262	293	240	200	195	226	256	186	234	310
217	194	261	235	273	277	198	185	212	304	197
202	269	204	317	246	181	345	260	344	208	270
208	339	331	173	267	154	273	175	300	295	279
279	307	306	289	214	244	318	186	309	186	298
241	999	199	301	277	214	251	136	137	298	218
277	324	217	200	342	364	136	327	769	737	196
273	335	240	230	233	275	232	225	285	272	210
214	269	194	303	288	168	276	263	271	276	269
208	138	242	274	301	286	219	204	69	193	195
160	205	141	152	183	173	297	190	261	140	284
266	204	142	205	224	225	259	226	193	283	116
183	199	241	216	273	271	197	277	335	248	291
269	210	354	330	320	254	286	288	244	64	237
300	244	189	280	283	64	247	238	290	188	185
198	0	254	235	294	290	228	283	305	234	187
344	146	309	241	268	252	270	314	265	269	244
260	263	190	284	237	271	258	184	225	307	195
169	255	285	218	244	253	243	233	235	211	362
228	231	266	264	282	88	221	160	225	282	275
15	315	216	328	326	231	296	186	326	237	272
223	292	270	341	255	266	294	287	237	353	274
270	10	180	346	335	324	173	291	319	253	261
711	284	359	283	291	225	276	260	187	219	283
255	224	250	299	301	288	329	268	117	310	224
266	216	254	286	275	179	312	121	332	307	277
192	240	300	308	327	333	335	299	277	255	

345

1985.5_1164EK03	205	211	164	169	158	210	159	250	333	119
198	281	146	251	183	208	177	208	122	195	172
375	253	372	225	184	219	203	201	249	280	255
232	230	175	237	336	218	328	215	176	288	200
179	180	234	166	200	171	263	224	196	157	309
258	309	303	316	231	125	296	198	303	234	313
182	281	346	318	241	218	189	342	177	262	159
198	177	174	191	398	214	222	217	173	278	275
281	251	293	180	235	175	244	279	251	284	261
282	227	196	207	237	239	210	146	168	293	296
394	260	263	292	202	261	189	152	556	155	238
233	199	999	240	244	192	332	153	268	234	255
478	241	177	963	251	192	226	290	177	197	222
293	166	221	225	235	243	212	228	210	277	212
206	209	170	287	278	202	248	303	313	223	277
229	255	272	244	263	269	255	368	295	432	373
490	279	413	458	208	475	296	488	230	235	177
183	148	208	186	227	159	322	273	117	289	202
114	252	229	245	220	206	193	287	410	191	282
164	186	209	275	281	153	179	216	182	165	269
117	308	205	165	193	178	163	173	210	193	185
204	158	228	158	223	188	257	205	289	284	27
294	219	169	141	226	279	204	266	208	309	203
234	125	116	256	197	199	225	178	275	162	243
149	240	226	193	334	157	191	261	248	118	354
170	303	279	295	206	0	315	264	302	269	307
319	237	280	236	163	136	275	103	284	252	271
325	288	172	257	178	288	182	302	139	247	266
235	101	172	273	236	214	191	201	224	283	282
232	305	187	227	305	183	142	159	218	177	194
121	185	269	213	201	209	360	308	184	254	158
289	213	190	214	333	176	267	216	244	230	294
151	145	289	334	331	332	328	342	307	274	

346

1991.6_2011EC38	276	249	118	345	344	269	318	212	575	292
281	350	285	357	419	393	300	367	452	325	278
454	255	477	269	223	398	306	295	518	385	528
496	494	415	495	634	176	590	334	306	273	353
279	312	726	288	213	335	297	197	264	271	685
314	580	572	576	283	288	567	337	688	250	447
318	706	468	457	264	324	292	449	370	339	265
327	362	249	472	390	461	173	413	478	575	617
640	545	608	237	645	139	665	541	673	702	534
703	659	637	91	658	198	648	238	269	690	697
341	754	764	737	313	480	190	496	356	503	792
566	301	240	999	900	607	257	255	300	401	591
311	350	297	301	284	175	95	326	271	279	228
296	205	334	436	370	337	349	405	368	450	433
421	515	450	572	584	423	541	494	607	557	600
453	107	313	575	517	526	232	443	259	459	450
444	387	441	461	109	304	324	470	506	100	338
427	401	130	259	261	318	602	207	212	351	138
270	362	643	205	439	326	311	449	458	482	255
290	187	249	321	293	381	286	310	367	178	481
201	676	191	269	256	62	279	248	673	305	190
454	0	461	275	296	235	344	303	529	590	41
224	147	319	465	218	655	212	384	522	765	447
317	362	255	258	384	198	341	165	526	279	790
165	475	618	384	512	273	185	418	224	261	547
260	601	583	294	191	250	664	271	630	116	668
360	678	137	678	236	407	765	179	788	349	631
536	903	199	599	314	238	200	320	245	604	617
372	154	384	705	696	658	348	519	574	272	255
214	318	511	536	538	537	325	378	540	391	593
390	379	525	508	484	439	424	578	339	556	407
467	380	173	394	543	196	482	176	540	552	550
292	365	287	355	323	337	165	367	294	286	



347

1997.0_1288EC09	260	251	120	334	340	236	322	214	540	254
282	324	278	329	362	380	268	331	430	352	307
429	241	442	260	201	392	324	304	480	389	473
469	470	384	449	614	165	574	312	327	293	353
288	293	672	288	191	337	295	174	255	276	634
293	588	567	573	294	284	563	333	652	244	439
321	677	463	442	259	308	303	433	333	333	257
303	410	246	461	366	470	177	374	465	541	589
608	500	582	276	612	129	634	546	636	669	512
670	622	605	95	619	165	609	259	252	703	710
339	705	709	688	319	614	208	494	346	496	839
709	277	244	900	999	727	260	263	297	383	553
325	344	282	297	316	144	98	329	261	258	278
297	202	349	419	366	361	361	433	396	456	468
377	488	410	591	602	424	549	484	603	567	608
430	126	301	577	529	542	261	438	256	429	447
410	381	418	443	110	289	315	447	508	128	348
399	372	127	249	242	322	570	202	144	327	123
289	379	593	172	402	328	334	427	422	442	230
277	151	248	342	312	365	267	259	350	160	432
241	636	163	265	281	61	298	247	624	293	186
420	0	444	254	310	249	321	263	531	590	41
214	105	321	417	207	605	166	352	510	723	439
311	391	258	255	353	184	334	149	491	270	727
165	423	552	351	531	260	185	373	211	161	518
266	612	547	266	188	230	626	328	593	138	583
392	608	114	622	211	435	718	178	741	344	610
561	930	186	604	304	234	155	302	298	599	574
371	125	381	672	658	614	324	461	524	244	247
188	299	502	504	561	489	326	393	521	385	517
398	365	487	491	493	433	413	544	299	518	388
452	380	158	427	541	193	497	158	539	560	572
278	371	282	326	299	309	207	332	252	277	

2014.0_1288EC06	256	258	57	266	296	239	284	231	391	209
289	323	293	318	401	383	256	379	376	338	252
329	255	357	241	236	335	309	250	360	292	353
364	354	327	459	470	3	444	259	244	290	321
257	294	534	229	161	305	276	212	283	262	654
238	443	431	435	239	266	429	289	434	244	335
279	418	345	341	260	307	285	336	311	304	218
287	363	222	364	323	401	160	340	428	382	392
426	353	404	246	417	159	340	424	330	538	358
541	325	323	125	334	184	332	230	229	593	601
307	377	370	421	242	777	219	367	308	371	660
873	214	192	607	727	999	229	218	231	321	458
296	284	227	266	267	121	123	274	230	212	171
266	161	258	336	291	311	285	350	351	436	430
307	367	299	414	414	404	380	435	432	419	422
329	87	264	398	408	403	207	375	263	382	394
355	314	350	364	101	303	286	393	416	91	290
433	338	99	252	229	284	407	225	86	326	143
295	368	549	233	406	327	277	397	353	475	208
271	85	258	310	241	338	257	225	332	182	437
235	493	113	245	237	4	295	253	503	236	148
393	0	354	266	252	199	258	236	404	441	0
242	130	273	355	234	449	159	299	396	459	353
286	371	242	240	331	203	348	84	358	257	576
126	336	405	314	402	269	138	303	182	138	433
276	490	341	241	159	304	463	291	405	171	372
340	323	92	348	175	443	413	264	406	283	486
445	670	169	385	267	206	105	245	302	372	482
310	95	287	389	352	345	224	389	368	226	207
172	227	360	351	433	335	246	257	419	284	348
356	299	390	339	317	324	382	436	258	401	379
421	317	149	334	471	213	388	166	410	398	401
214	346	256	276	255	291	200	313	244	218	

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257	246	263	196	170	193	199	180	104	326	263
329	214	293	202	144	229	267	282	314	321	220
301	269	219	240	292	113	280	244	251	302	205
156	211	260	224	236	303	282	289	262	247	277
347	290	273	271	271	190	272	364	282	300	256
323	302	291	258	256	332	244	274	206	264	217
266	218	262	239	329	405	255	212	273	334	248
237	227	269	137	223	255	272	286	274	300	226
287	269	266	199	271	239	295	327	238	293	301
544	258	259	277	321	263	237	276	369	277	227
242	251	332	257	260	229	999	296	304	303	244
613	314	272	344	237	197	189	244	268	212	209
969	198	304	339	315	331	313	387	417	406	352
271	241	230	252	266	319	263	258	284	302	262
401	139	222	224	268	267	325	258	117	316	288
223	57	286	257	162	231	347	355	255	137	238
165	233	267	200	230	250	315	250	79	254	99
214	111	227	49	157	204	143	236	305	147	176
175	149	187	257	284	194	222	266	104	0	216
203	262	134	82	207	115	136	186	219	202	243
129	224	199	129	274	194	336	138	169	311	1
228	191	244	152	203	262	153	230	207	271	315
213	79	218	156	157	239	221	102	173	172	184
182	230	213	172	226	203	256	251	235	0	240
185	172	302	229	212	94	242	224	232	216	276
220	191	213	246	220	239	254	217	276	308	293
241	249	244	290	176	282	92	223	250	259	204
237	3	183	287	234	198	201	133	268	294	291
255	232	215	223	240	255	287	219	199	244	109
122	270	231	320	244	340	356	242	67	135	209
190	328	140	200	293	181	206	205	251	240	211
240	176	310	287	323	311	288	341	340	241	

2075.8_2011EC34	267	295	162	283	300	327	308	245	233	247
186	284	737	270	226	259	272	210	152	338	293
287	167	261	559	234	227	561	350	290	327	248
304	271	222	238	243	166	211	366	331	338	147
177	677	298	253	187	257	240	233	353	766	256
288	267	226	252	253	229	246	336	220	280	206
325	205	237	212	311	257	775	232	181	288	240
270	223	493	217	225	256	170	267	221	254	218
199	219	213	247	181	153	203	258	203	251	211
250	203	192	174	185	206	189	899	499	232	230
255	221	221	217	278	188	199	219	286	218	223
194	136	153	255	263	218	296	999	261	318	277
279	283	246	177	257	449	181	290	206	184	152
271	450	223	226	234	266	220	214	235	280	256
190	202	219	223	211	234	204	202	230	228	226
228	182	221	243	224	207	154	198	86	203	274
218	158	199	227	161	208	322	202	266	174	288
267	196	139	822	315	308	272	287	241	314	194
699	204	279	238	247	288	146	304	290	288	315
246	562	336	365	282	158	380	396	232	141	269
179	258	250	213	332	236	175	479	287	266	186
187	29	263	178	269	253	297	258	235	245	0
213	114	225	286	275	200	252	307	279	211	272
266	197	322	244	239	652	304	478	211	258	273
665	218	229	224	247	293	453	218	234	88	286
168	248	258	237	648	191	216	267	192	206	275
0	166	257	206	492	247	205	193	209	276	232
222	231	775	217	247	220	369	239	755	220	241
292	136	749	243	191	314	587	437	358	217	249
162	236	315	257	269	199	119	225	214	200	278
242	208	212	241	164	245	319	237	152	182	231
250	248	97	210	264	237	278	233	237	218	232
209	238	252	264	238	274	295	300	310	215	

2086.8_1344EC29	363	277	188	251	247	329	231	251	394	155
196	274	320	334	312	326	179	259	289	352	324
275	215	350	353	211	341	342	314	367	356	364
361	364	314	402	385	172	379	335	261	248	137
193	293	368	256	205	359	237	358	233	274	334
350	306	332	315	207	290	317	330	326	314	256
316	351	287	252	302	284	264	275	288	333	240
299	321	259	248	387	330	325	194	295	331	259
284	280	287	244	273	275	311	354	311	371	285
382	304	284	199	294	313	314	295	262	375	375
316	274	278	308	325	274	122	310	342	312	271
208	137	268	300	297	231	304	261	999	344	315
340	383	230	278	237	269	198	252	228	102	201
310	318	263	315	297	304	240	328	308	378	269
274	263	245	313	311	253	310	276	307	320	302
185	178	191	292	316	300	254	260	164	238	266
287	168	247	226	160	215	368	249	265	193	273
414	326	487	265	334	231	419	256	186	290	128
298	345	368	249	288	307	280	409	360	220	315
407	247	330	382	313	299	280	266	323	123	385
86	431	165	263	334	102	170	299	300	282	190
283	480	257	196	274	234	341	223	361	321	26
304	237	309	325	170	375	263	336	398	377	384
217	307	179	229	296	296	328	191	290	264	332
228	351	255	280	321	318	251	276	337	112	406
182	324	305	256	279	171	333	246	317	275	343
136	281	412	339	283	365	293	200	319	362	394
321	342	250	360	255	306	287	262	285	357	292
297	46	322	308	277	339	323	353	397	310	282
174	246	344	329	307	313	252	283	283	276	376
236	249	313	270	281	291	399	331	203	395	236
291	244	112	307	314	167	326	260	323	342	299
248	240	334	311	304	374	359	376	347	233	

2089.0_1288EC05	325	363	195	370	357	356	357	262	341	277
	340	303	348	423	313	371	364	327	281	459
	405	297	365	384	277	402	381	370	377	335
	389	365	428	385	388	227	421	450	413	346
	260	407	342	312	178	391	342	286	351	392
	307	397	406	406	338	432	403	364	372	338
	332	376	395	406	332	401	375	396	312	320
	338	314	408	370	285	398	248	396	318	387
	379	372	390	380	388	240	396	387	393	452
	460	388	367	235	375	235	373	352	362	463
	292	361	367	380	329	366	286	400	292	379
	355	298	234	401	383	321	303	318	344	999
	327	355	330	269	349	400	221	320	349	322
	319	376	361	391	383	384	360	410	381	444
	326	387	377	424	419	413	413	397	417	434
	445	221	320	407	449	439	266	304	201	318
	283	237	294	274	271	281	389	348	383	217
	558	314	128	316	341	357	359	255	220	373
	314	323	409	253	354	403	260	385	427	260
	378	308	348	358	284	296	415	418	331	187
	314	439	309	263	392	194	260	277	342	332
	315	0	401	300	446	337	306	321	372	419
	264	144	458	378	349	395	284	439	313	395
	309	204	301	347	285	384	296	294	346	354
	263	355	408	232	350	323	387	316	370	229
	257	376	432	341	349	189	397	284	401	226
	297	367	152	342	359	348	378	221	372	336
	365	372	346	421	360	360	311	393	419	398
	344	223	350	409	379	439	356	408	461	364
	272	379	455	383	337	348	289	324	331	366
	317	305	471	408	407	384	401	454	278	379
	413	387	253	375	432	217	386	244	446	398
	375	341	388	441	384	396	285	422	403	334

2091.4_1288EC40	254	242	165	310	296	231	289	263	445	215
227	256	252	282	382	389	258	338	405	330	316
348	224	366	219	203	349	262	264	342	317	347
353	352	404	487	628	231	586	317	271	246	319
240	303	436	259	161	312	264	253	262	280	471
285	582	575	579	228	276	574	317	620	251	369
302	587	386	379	235	371	237	370	246	344	245
346	387	217	452	351	453	234	350	488	517	573
572	525	575	218	573	191	529	507	556	633	516
630	549	537	193	546	208	555	241	266	660	668
276	554	563	636	270	466	172	417	269	424	509
460	218	255	591	553	458	244	277	315	375	999
300	302	269	294	261	130	204	265	224	226	233
269	168	418	461	420	422	441	458	432	475	454
600	496	417	582	573	394	512	534	566	519	546
380	194	301	501	471	490	237	415	293	440	435
393	407	425	454	204	348	357	464	479	220	324
323	329	96	240	221	289	467	252	113	268	120
263	397	352	203	385	350	369	401	348	289	222
290	188	234	271	258	354	247	251	341	142	483
157	547	213	268	231	83	237	234	430	273	131
512	4	428	247	267	243	309	295	451	601	95
219	188	315	368	252	588	169	373	414	615	466
275	309	281	244	349	192	345	197	542	271	517
144	429	530	344	565	258	188	406	228	231	561
283	610	458	287	162	221	598	394	567	221	453
394	478	108	517	246	403	602	211	617	306	540
581	596	202	537	338	229	162	323	203	504	952
373	128	303	537	508	476	248	457	484	241	216
214	314	472	426	522	501	322	422	515	430	384
440	506	575	474	455	452	385	558	315	434	427
500	472	142	360	577	227	487	194	518	496	667
294	415	278	299	303	284	242	330	276	290	

2101.9_1164EK03	205	304	147	283	301	260	284	238	357	166
251	284	273	267	260	253	239	241	220	332	273
360	248	382	234	226	307	303	318	320	360	290
306	289	305	387	372	170	346	264	289	319	255
236	289	309	269	258	359	274	265	287	289	369
342	351	335	327	309	241	329	320	338	240	338
297	351	350	342	247	311	286	337	276	276	281
265	272	284	287	509	399	261	230	303	342	319
322	301	340	158	311	281	325	327	330	375	295
344	311	292	213	320	272	304	325	274	354	360
870	316	315	332	364	344	289	319	660	330	291
299	277	478	311	325	296	613	279	340	327	300
999	335	236	498	305	213	215	290	328	318	170
628	212	280	330	304	316	285	350	367	417	313
315	299	256	303	307	354	301	280	359	351	349
397	190	229	297	311	317	315	388	193	457	405
394	246	434	404	181	353	376	509	311	226	308
279	295	235	192	253	284	358	242	151	317	109
243	181	296	204	222	256	222	286	364	161	231
270	202	245	323	270	253	256	299	210	176	332
222	306	115	167	267	147	231	212	263	266	246
200	240	255	167	285	220	327	253	257	353	22
277	170	275	170	236	305	209	288	296	349	337
225	214	213	266	210	245	216	202	278	276	225
182	296	294	172	276	200	257	314	309	168	334
179	266	337	236	257	199	332	249	301	240	303
259	213	238	279	282	269	330	243	330	332	357
291	301	267	320	248	274	206	253	271	289	276
239	184	234	321	244	260	180	218	297	323	325
294	249	277	247	343	279	306	229	232	272	229
213	275	284	348	291	292	354	287	137	237	273
241	304	188	257	312	153	259	241	295	285	285
255	217	356	371	331	367	321	382	355	260	



2127.8_2011EC19	317	404	171	296	317	371	305	194	329	186
272	294	309	368	257	272	277	211	228	364	277
327	237	391	307	241	319	372	308	360	334	320
381	354	263	289	352	189	319	338	381	351	254
206	318	380	298	287	340	308	335	338	306	325
311	361	353	351	341	347	355	304	331	283	327
274	341	375	333	273	324	304	357	257	254	309
247	275	318	270	348	377	337	291	293	360	321
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388	366	375	199	373	258	376	322	337	382	388
302	304	312	335	292	317	345	356	301	359	307
326	324	241	350	344	284	314	283	383	355	302
335	999	302	304	415	313	185	316	335	330	200
346	342	296	320	299	306	289	337	322	392	306
274	306	229	375	368	339	350	305	338	361	361
315	173	238	318	344	348	257	251	108	246	276
156	118	257	227	180	183	321	276	304	177	285
338	269	227	234	361	305	321	170	178	356	154
256	219	327	194	206	283	178	307	375	299	343
331	221	389	351	278	247	293	365	212	33	304
213	327	123	170	380	112	187	256	301	291	287
257	125	261	199	319	237	277	286	247	365	135
319	135	378	165	259	331	276	277	243	340	357
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256	324	328	171	296	189	301	267	291	152	377
239	212	336	248	301	140	318	259	293	176	363
214	285	163	275	326	255	315	196	321	274	376
269	342	318	385	206	322	279	282	292	353	268
259	120	228	337	298	394	252	273	400	333	318
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187	261	268	332	334	309	325	292	147	269	294
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271	228	328	361	338	356	277	327	314	280	

2135.1_1344EC07	264	276	263	231	253	243	312	225	285	304
277	268	296	351	289	276	282	301	249	266	248
282	199	297	314	236	274	272	305	306	310	283
294	294	263	276	295	297	364	329	300	290	241
252	321	264	268	200	276	280	269	256	262	260
248	199	224	209	268	302	209	242	274	221	192
227	279	255	195	256	256	229	209	240	240	298
267	245	276	254	228	340	297	218	274	240	204
213	246	246	228	237	328	269	241	273	253	242
254	251	227	279	242	177	235	200	271	240	235
196	273	279	294	196	224	224	233	247	229	301
179	217	177	297	282	227	272	246	230	330	269
236	302	999	171	198	258	267	279	271	224	217
300	271	203	245	220	243	172	246	241	351	269
265	201	264	251	254	211	235	238	239	262	253
421	290	234	243	229	217	227	220	243	256	215
138	282	194	262	338	188	288	137	263	299	255
373	336	200	316	256	312	305	242	282	304	264
233	249	263	298	311	289	209	303	295	259	338
298	241	295	316	279	271	334	293	282	94	261
208	295	263	223	287	60	250	241	306	254	182
258	146	297	267	285	293	289	255	241	219	23
244	252	327	284	254	283	270	286	263	273	258
243	284	221	309	281	238	246	205	241	322	257
123	309	318	162	259	241	255	257	294	283	300
256	262	197	257	259	184	232	207	278	296	256
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248	306	270	257	227	305	281	275	292	275	299
273	92	249	278	253	292	184	297	268	308	298
149	269	287	241	283	225	298	219	269	173	332
251	249	264	234	268	256	330	277	210	295	256
271	277	200	255	272	194	262	186	247	227	227
258	288	340	379	339	314	233	288	276	254	

2139.0_1164EK03	233	237	145	178	198	234	164	259	367	131
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369	263	403	228	227	249	249	250	294	310	301
282	277	238	288	368	212	357	233	214	307	218
231	251	318	264	175	175	271	258	240	190	387
297	335	355	346	252	215	329	250	340	226	355
217	332	390	367	243	254	210	388	223	258	245
252	259	191	256	467	252	238	235	226	291	300
299	277	315	239	262	208	284	319	292	350	278
351	261	234	207	271	255	244	191	231	355	356
446	284	288	325	295	305	215	221	605	224	281
279	200	963	301	297	266	344	177	278	269	294
498	304	171	999	308	195	180	328	188	230	212
357	185	245	264	254	253	218	258	257	352	234
250	252	206	330	324	265	294	322	323	298	312
264	194	240	281	294	309	285	392	293	429	395
466	309	429	462	186	454	335	512	279	193	229
268	260	206	180	257	164	372	258	104	328	172
184	292	271	235	284	218	238	298	423	238	265
229	193	250	308	285	210	240	242	262	23	308
130	356	229	208	238	169	253	165	283	289	160
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272	243	242	230	286	347	212	296	263	345	277
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198	360	312	237	196	172	334	245	314	287	337
311	280	244	282	202	250	289	150	317	328	326
346	339	201	316	220	288	206	269	191	323	299
268	172	204	305	260	280	188	259	284	301	287
251	272	223	231	342	234	256	207	265	205	264
242	223	314	251	241	232	377	337	231	291	273
316	292	200	280	347	156	297	241	287	281	329
224	237	324	337	340	366	335	376	335	278	

2174.2_2011EC19	330	289	184	338	347	324	325	157	292	237
227	368	262	380	301	333	327	339	272	403	276
448	165	370	338	246	340	329	368	316	554	307
322	303	278	300	298	199	346	341	371	607	218
243	326	353	289	209	321	474	206	327	302	330
329	285	314	296	555	328	303	241	294	215	353
233	296	358	352	240	267	319	316	247	248	426
228	252	332	250	300	311	217	257	278	296	307
289	267	312	392	313	189	303	275	322	328	255
324	282	266	202	311	168	275	224	412	328	331
226	243	244	287	330	344	368	221	299	226	285
288	342	251	284	316	267	237	257	237	349	261
305	415	198	308	999	353	192	612	359	374	167
268	361	268	272	284	278	255	280	294	313	263
278	279	241	310	296	246	299	274	319	316	310
267	187	223	235	313	304	230	206	151	236	253
261	136	212	240	160	263	341	257	258	164	339
373	325	125	257	334	325	326	172	223	429	27
245	280	283	254	328	316	204	239	490	206	316
340	258	419	402	527	302	504	355	230	78	295
655	250	260	324	342	413	230	249	320	297	200
234	0	242	173	416	399	350	359	239	329	63
375	97	401	265	365	298	224	427	238	337	334
249	234	182	291	195	306	216	185	265	394	228
181	272	408	107	273	239	300	260	255	207	392
165	245	318	215	334	150	263	179	229	256	345
183	253	189	292	406	282	271	109	329	298	360
255	322	325	317	208	290	309	250	281	297	231
316	30	222	328	261	330	207	324	344	299	293
365	227	329	297	261	247	236	232	187	209	296
283	236	253	333	306	304	397	324	160	243	257
278	247	160	287	296	188	286	211	320	313	297
218	278	338	342	334	348	275	333	324	240	

359

2197.4_1344EC14	324	367	210	312	326	335	366	143	181	281
329	280	468	337	172	218	328	197	123	406	301
359	248	195	465	275	259	417	329	318	349	202
302	262	149	152	166	218	223	451	352	346	269
271	473	181	256	197	369	363	249	377	580	165
265	266	272	278	340	391	277	315	151	267	267
304	154	282	260	288	264	552	266	247	149	334
157	151	601	179	199	273	224	307	197	321	235
249	298	249	319	257	261	248	170	254	176	296
186	255	253	223	261	188	254	463	566	195	214
165	158	156	144	243	237	318	233	204	231	166
218	364	192	175	144	121	197	449	269	400	130
213	313	258	195	353	999	212	310	427	390	222
203	660	248	249	269	283	246	289	311	272	217
135	143	249	211	215	211	210	137	217	246	220
231	182	241	160	225	214	197	132	76	160	177
87	133	159	160	187	115	301	182	191	177	275
274	216	164	495	324	366	193	165	222	268	235
434	187	191	166	178	327	89	242	323	113	355
286	474	387	319	337	188	426	463	120	43	171
309	181	240	268	327	225	267	478	182	271	193
172	0	145	297	408	350	234	534	194	279	140
297	78	409	221	279	148	280	284	136	137	268
198	116	212	332	181	618	145	423	105	326	147
477	313	220	70	110	165	624	123	252	205	281
172	71	266	261	676	90	221	93	210	57	236
0	260	126	178	579	121	121	155	130	200	280
113	144	594	229	151	319	462	279	532	192	114
179	4	415	267	216	342	431	316	379	307	312
271	274	436	240	117	190	228	202	145	221	195
89	118	207	280	294	291	301	160	70	143	212
124	244	86	206	174	190	165	98	199	147	117
183	105	270	310	253	248	148	275	253	183	

360

2200.0_1135EC03	194	246	714	175	172	118	170	146	156	154
294	104	177	178	197	178	165	239	253	258	110
153	221	146	163	299	152	196	120	158	199	62
186	132	232	156	76	814	313	130	194	230	279
224	184	137	183	173	218	209	175	188	180	175
186	203	179	183	198	137	186	166	32	165	198
191	122	240	215	182	238	197	229	344	208	246
204	272	223	218	211	307	198	191	310	191	118
151	107	133	5	118	299	209	223	218	202	115
227	205	161	935	297	217	256	338	190	278	267
100	101	64	94	218	221	173	249	228	243	313
248	136	226	95	98	123	189	181	198	221	204
215	185	267	180	192	212	999	241	448	118	263
209	188	254	224	272	279	224	266	205	251	277
300	165	158	215	206	288	217	156	189	220	195
245	952	123	207	213	207	303	166	63	206	221
118	16	139	0	890	161	298	190	233	913	156
108	193	306	248	164	170	119	87	166	59	247
164	2	208	279	217	171	0	0	124	85	176
90	178	115	110	178	264	297	186	184	143	67
136	78	240	64	87	219	210	60	96	108	126
118	130	119	221	225	209	196	139	58	183	46
221	136	152	144	83	135	178	189	152	46	259
108	21	6	411	177	216	87	138	82	237	63
154	222	34	0	122	4	195	49	212	207	217
250	119	164	164	201	159	50	27	109	106	128
0	166	84	45	198	129	75	223	62	75	197
94	180	141	79	206	321	197	253	178	102	141
93	0	41	297	76	74	113	32	105	295	301
1	265	237	149	86	226	104	62	132	99	23
94	147	284	58	262	53	293	99	99	227	207
79	176	4	101	220	102	187	209	111	56	72
257	104	281	334	209	188	213	189	151	168	

2206.1_1164EK04	328	251	139	433	352	290	394	174	382	357
284	280	279	357	317	372	368	333	285	392	430
581	161	392	356	266	292	325	575	275	685	268
302	287	271	354	364	127	294	308	464	553	261
248	292	337	479	195	321	457	238	288	286	343
525	354	350	343	475	322	344	281	373	222	352
258	385	349	347	281	277	278	347	251	277	365
258	268	323	313	288	312	200	239	320	338	338
322	304	357	395	355	201	309	268	333	356	321
374	309	326	246	351	109	327	258	375	342	347
281	275	275	312	538	347	246	262	257	269	279
306	327	290	326	329	274	244	290	252	320	265
290	316	279	328	612	310	241	999	323	394	172
268	287	268	297	302	306	289	320	305	332	294
281	276	304	308	291	326	303	253	305	288	299
314	231	173	241	328	305	230	282	86	302	268
308	120	279	280	106	281	285	318	240	153	419
334	311	97	266	303	394	394	180	288	343	19
298	322	309	248	330	342	370	294	570	164	189
386	86	402	395	659	332	420	334	279	206	314
518	273	316	224	407	426	257	185	294	529	176
187	0	216	246	371	384	564	303	271	376	2
220	94	407	243	340	322	106	406	310	348	326
162	265	222	211	215	304	263	171	357	355	261
200	307	369	249	230	236	285	249	169	12	404
119	247	288	179	322	238	324	234	354	84	243
3	288	165	317	363	311	295	300	309	569	358
244	345	255	315	219	171	205	173	241	320	277
238	143	202	279	276	311	205	273	322	195	199
324	166	293	335	232	276	202	223	275	231	212
227	275	313	305	262	306	305	277	149	275	217
252	285	45	283	249	207	315	105	315	301	263
191	196	230	246	159	249	177	235	203	222	

2225.2_1179EK02	306	338	340	237	264	291	295	195	289	226
199	348	274	268	278	254	247	253	277	294	330
372	283	300	297	267	329	314	285	280	368	293
290	289	286	296	281	371	354	294	351	363	190
230	273	283	264	223	371	328	249	301	325	293
246	230	247	237	364	392	230	216	289	222	240
218	269	269	254	241	219	263	252	182	267	325
236	291	280	210	240	253	254	198	242	278	235
233	265	244	360	235	223	292	338	278	265	274
267	263	251	450	274	246	269	261	335	304	293
292	280	280	278	272	229	338	196	295	193	314
204	769	177	271	261	230	268	206	228	349	224
328	335	271	188	359	427	448	323	999	884	316
285	363	216	205	212	220	203	227	246	320	188
234	258	223	304	314	258	295	267	305	305	304
225	455	286	300	305	309	209	210	235	212	210
172	257	182	195	431	279	364	220	277	441	267
353	272	185	243	276	295	307	246	241	343	204
256	225	288	307	294	269	282	250	402	281	324
299	274	364	368	328	247	294	300	247	132	242
318	272	212	287	396	48	248	284	295	263	226
276	102	274	227	290	313	266	335	349	267	164
338	264	398	319	319	324	289	295	289	289	249
367	280	264	385	244	339	284	284	270	348	226
261	309	283	211	315	299	301	257	313	259	379
255	332	246	306	323	247	249	273	260	282	283
199	261	173	295	335	254	288	215	292	270	304
326	265	289	334	275	339	325	352	299	341	233
271	137	229	334	277	288	228	348	303	343	350
826	352	348	292	374	208	206	240	222	280	308
271	237	281	290	311	246	387	305	218	330	235
287	243	244	293	280	191	332	252	323	332	319
253	267	348	363	343	355	328	324	309	286	



2226.4_1164EK04	337	303	19	311	262	301	277	202	274	257
149	355	265	238	224	225	243	190	281	306	370
463	236	309	299	220	316	265	370	278	431	300
282	285	276	230	248	1	266	309	353	392	150
169	249	314	305	183	320	226	217	290	313	246
328	248	250	265	343	372	258	209	288	184	258
234	247	297	274	225	220	295	269	191	283	298
226	256	319	257	197	268	219	197	234	300	235
241	284	254	372	243	47	260	303	270	269	289
273	287	259	103	260	98	280	217	289	296	292
298	224	225	262	316	172	291	189	310	189	226
172	737	197	279	258	212	212	184	102	322	226
318	330	224	230	374	390	118	394	884	999	160
237	340	235	190	228	240	205	219	248	263	226
192	218	250	278	283	220	263	239	280	258	284
237	87	259	281	304	289	125	208	178	219	218
139	203	160	187	74	211	286	217	261	88	306
312	211	136	279	294	277	307	281	267	355	164
191	252	255	248	181	313	278	277	438	231	283
333	187	401	396	385	248	273	287	258	67	244
292	268	203	256	345	53	208	250	326	316	164
220	0	288	236	301	296	356	335	329	250	184
281	77	382	289	248	301	243	288	283	283	268
279	279	295	287	223	300	286	243	255	299	255
210	293	266	245	296	254	276	258	254	154	378
214	285	252	298	287	153	282	249	290	227	249
25	248	158	269	329	230	245	223	249	340	307
302	263	281	285	133	218	272	280	263	339	233
303	141	222	256	228	284	216	297	281	262	303
853	279	355	310	364	261	197	291	260	274	251
276	248	298	266	270	249	329	292	163	226	265
264	237	88	280	281	125	337	4	326	306	295
167	255	249	268	268	301	320	281	235	218	

2233.1_1313EC75	170	218	229	225	233	129	202	132	164	175
270	246	151	247	237	217	193	288	265	236	103
198	335	219	124	256	264	172	233	168	214	150
172	157	244	189	139	253	219	234	152	179	248
232	201	156	161	111	208	186	176	212	217	195
170	187	189	182	194	152	183	203	198	204	177
201	210	195	179	166	239	172	190	274	200	251
198	253	206	273	195	299	182	272	295	205	128
175	163	133	124	130	182	233	255	251	240	169
248	212	223	267	257	167	238	201	198	274	270
146	220	209	196	187	209	185	312	209	303	201
194	196	222	228	278	171	209	152	201	249	233
170	200	217	212	167	222	263	172	316	160	999
206	234	166	211	201	209	189	237	198	224	260
217	208	198	207	206	253	204	211	173	184	148
194	265	212	233	199	198	154	228	129	157	276
146	34	238	112	272	191	312	196	188	296	223
257	245	232	96	164	202	151	116	169	247	222
144	171	175	282	328	165	144	270	214	112	261
147	145	184	220	155	248	264	251	200	81	173
124	203	192	116	181	13	195	169	153	150	156
293	0	241	242	233	150	160	177	130	165	61
179	138	165	171	161	234	215	259	155	187	258
150	210	195	313	133	206	175	187	238	232	123
114	248	153	8	205	167	163	237	265	257	264
226	161	307	209	172	241	133	84	141	134	265
0	188	110	170	156	214	183	196	205	160	271
159	296	163	195	168	386	220	305	204	169	177
167	40	107	291	175	145	137	149	223	368	353
65	268	202	159	190	212	180	134	129	142	177
182	202	251	170	215	183	405	253	182	221	177
141	140	60	130	238	100	161	269	193	172	155
211	128	422	417	367	361	321	418	330	278	

2253.1_1164EK03	231	298	145	247	255	234	253	238	360	183
239	269	266	247	244	222	187	218	216	324	271
325	220	330	233	209	268	294	314	343	336	280
331	304	257	271	309	193	309	264	276	319	236
211	251	321	289	219	329	292	300	285	273	332
356	322	304	304	298	213	300	372	302	292	277
330	315	330	277	257	340	256	290	259	273	245
281	256	279	273	373	407	292	203	298	334	285
269	249	289	172	258	288	277	305	278	336	242
330	278	276	224	288	254	300	330	258	336	342
564	274	274	289	329	274	230	288	395	286	268
254	273	293	296	297	266	969	271	310	319	269
628	346	300	357	268	203	209	268	285	237	206
999	210	305	353	318	340	315	391	426	443	365
285	262	285	291	299	328	288	289	314	333	286
418	194	209	259	296	296	320	291	172	329	312
268	140	303	288	201	232	379	368	295	232	284
272	296	232	185	261	253	365	232	123	278	135
243	167	278	173	231	208	220	284	320	232	237
206	226	256	283	274	247	269	265	186	107	283
190	305	115	156	245	112	233	201	272	284	248
194	175	256	183	294	227	347	180	208	327	155
248	158	266	219	225	336	192	264	259	298	340
227	164	221	220	208	258	240	198	252	235	245
179	268	269	189	289	225	262	267	296	155	303
221	225	314	217	240	141	284	225	261	247	309
207	235	218	266	256	248	273	205	294	322	319
250	296	286	316	229	275	183	234	278	295	257
277	130	190	315	247	270	219	209	301	324	298
258	236	271	256	286	285	332	221	253	248	193
196	267	262	357	286	345	408	288	103	215	253
260	330	156	263	335	173	267	244	293	285	258
269	234	343	342	331	349	332	355	354	255	

366

2255.2_1344EC14	371	322	206	473	483	414	385	136	198	293
334	268	469	386	238	245	344	209	162	342	361
355	293	232	537	289	249	444	331	284	341	224
292	259	166	180	172	200	256	549	342	348	296
348	490	234	304	175	361	359	247	403	545	191
287	247	260	257	332	396	262	263	167	250	282
274	186	282	280	299	229	489	269	208	152	409
161	187	585	199	226	281	203	321	196	267	233
210	262	234	253	245	213	269	209	285	206	258
212	270	261	197	257	164	264	481	587	210	217
174	153	152	155	277	234	364	212	199	218	189
235	335	166	205	202	161	198	450	318	376	168
212	342	271	185	361	660	188	287	363	340	234
210	999	258	253	278	294	283	296	295	264	237
193	176	221	234	222	203	228	147	213	241	216
215	163	239	161	237	225	195	152	56	167	173
150	111	176	142	188	183	248	218	177	167	432
275	214	203	474	405	385	183	70	283	304	234
444	186	195	190	157	286	110	253	336	159	444
398	521	473	401	304	149	458	481	135	96	197
298	177	212	209	324	224	324	457	223	289	172
159	0	162	281	440	309	225	364	163	291	194
250	140	412	164	302	201	360	297	187	173	267
196	136	213	374	187	580	153	389	171	394	144
471	254	239	89	141	184	572	133	208	257	272
176	116	285	235	566	68	199	102	172	61	228
0	230	87	184	553	141	155	153	158	228	273
128	155	563	256	136	284	434	273	484	184	151
199	4	391	252	181	309	428	342	372	276	298
231	271	417	234	133	197	236	243	187	229	215
164	172	196	337	337	276	253	163	7	171	186
164	252	34	178	182	134	162	77	216	150	148
216	109	304	293	273	243	114	248	240	221	

367

2313.9_1344EC18	246	256	202	266	251	236	279	508	384	233
243	271	263	297	291	346	250	271	293	315	283
342	237	359	234	279	349	258	264	366	303	356
372	379	359	329	458	267	431	286	273	276	275
235	281	318	248	185	342	287	222	213	242	331
263	380	418	402	255	252	402	490	462	515	331
496	436	327	328	530	546	236	305	319	604	247
754	340	253	351	302	360	206	323	304	342	385
388	379	415	206	403	194	446	417	439	417	379
435	434	431	275	412	260	424	219	235	436	437
273	435	439	449	266	323	238	326	257	314	360
297	240	221	334	349	258	304	223	263	361	418
280	296	203	245	268	248	254	268	216	235	166
305	258	999	681	975	982	958	938	926	746	848
707	380	255	423	448	320	401	361	399	360	399
271	250	259	420	431	437	295	252	185	275	254
315	294	258	261	284	300	342	309	356	280	270
343	353	192	240	231	279	398	516	207	253	157
274	340	324	270	330	326	255	304	363	217	274
313	222	346	371	234	338	302	283	386	138	341
187	440	240	210	265	137	229	222	311	259	149
311	175	334	224	275	231	283	383	391	431	44
258	262	289	322	227	425	275	355	369	456	503
271	344	341	257	343	194	617	213	412	263	385
160	346	392	354	395	655	196	288	295	312	433
258	443	430	280	193	276	426	319	406	214	408
214	430	190	421	252	375	445	172	442	304	470
414	388	195	384	470	304	252	275	239	371	408
577	564	243	388	394	386	184	326	357	312	309
201	306	353	275	395	580	679	971	410	904	351
800	658	410	331	344	908	394	411	262	358	615
354	766	754	355	388	191	422	203	435	437	422
440	641	396	423	355	471	312	389	350	304	

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2318.9_2011EC23	256	277	173	250	241	244	238	525	448	219
234	254	267	300	315	395	234	328	320	294	300
359	238	366	273	311	386	305	258	414	347	403
386	387	370	391	545	216	513	348	250	272	285
221	306	374	276	196	326	281	278	259	258	346
281	452	499	491	257	302	492	542	522	588	314
546	495	337	322	581	583	232	338	323	670	280
735	355	250	402	308	389	292	402	375	438	465
485	486	494	241	498	204	493	472	494	514	476
512	479	466	242	477	273	472	214	243	457	459
315	471	478	553	257	391	204	359	302	367	393
360	230	225	436	419	336	339	226	315	391	461
330	320	245	264	272	249	224	297	205	190	211
353	253	681	999	704	684	696	737	665	697	737
724	421	372	418	438	396	411	410	479	413	460
359	252	312	461	441	453	288	318	274	298	321
341	297	310	305	275	284	391	346	401	278	290
311	344	206	214	222	238	449	535	177	245	172
270	405	332	293	358	355	270	361	387	188	287
251	265	265	329	281	345	293	292	351	141	394
186	537	221	243	266	157	210	260	362	270	185
361	185	371	222	265	276	293	479	470	498	165
345	346	322	372	316	535	294	405	428	517	540
338	303	327	308	413	252	681	273	444	288	446
230	456	467	354	379	654	236	306	328	261	510
275	467	473	319	210	283	513	333	529	266	469
203	422	204	450	271	364	503	221	515	309	494
442	437	219	435	539	347	308	342	243	435	468
761	848	247	460	473	485	279	372	472	377	337
167	358	443	407	439	870	495	665	436	703	390
642	662	470	434	423	730	459	469	329	425	721
399	765	742	340	446	194	431	291	457	451	450
571	698	397	484	394	466	331	425	407	369	

2322.8_1344EC17	252	263	228	271	273	221	259	532	407	218
227	284	300	302	301	359	235	282	296	296	258
357	233	375	246	299	360	327	293	379	313	366
376	384	392	341	469	291	458	283	275	305	264
266	305	352	247	174	328	309	249	209	282	362
277	420	458	444	261	258	443	497	474	525	333
518	455	352	331	549	562	247	311	327	628	273
756	338	243	379	322	375	229	307	297	356	397
402	387	434	207	418	216	461	433	455	433	399
452	447	443	318	430	256	441	230	256	452	453
333	456	462	461	280	337	232	329	274	318	370
296	233	235	370	366	291	315	234	297	383	420
304	299	220	254	284	269	272	302	212	228	201
318	278	975	704	999	974	958	957	923	744	847
719	398	282	432	459	332	418	381	420	379	399
317	273	291	430	445	450	299	245	221	255	249
362	297	293	272	287	320	355	319	374	289	300
355	372	213	239	219	259	422	547	209	269	159
299	344	346	272	333	298	253	321	382	290	304
305	254	348	384	243	334	307	305	398	81	370
238	472	235	213	283	192	262	222	352	260	120
332	158	380	235	283	243	304	384	412	448	149
298	257	300	340	272	455	283	380	384	469	528
321	344	339	275	345	229	642	264	416	287	389
197	366	374	325	408	663	228	301	319	299	462
255	447	425	295	213	246	455	324	448	230	414
212	460	184	452	270	348	448	195	448	326	476
423	395	211	399	482	331	310	323	243	391	420
605	598	243	427	423	402	193	317	378	332	330
193	349	367	308	401	605	679	961	421	922	367
797	653	434	350	365	916	440	437	274	411	633
377	747	768	358	416	208	440	274	448	445	426
447	619	411	457	391	503	321	415	391	326	

370

2330.5_2011EC22	253	264	231	267	257	246	287	507	389	238
253	260	310	310	292	339	255	286	291	296	285
340	229	360	266	300	349	313	287	356	289	341
360	364	349	331	442	290	439	294	284	327	283
261	304	313	233	191	329	304	266	226	280	337
240	395	444	430	275	256	427	499	451	521	340
515	427	343	337	545	542	250	321	320	608	257
742	340	265	388	331	372	241	317	319	336	372
377	377	406	209	395	212	441	409	442	416	382
435	438	419	297	403	255	412	245	268	438	440
302	438	440	441	268	374	228	305	278	294	363
343	275	243	337	361	311	331	266	304	384	422
316	306	243	253	278	283	279	306	220	240	209
340	294	982	684	974	999	952	937	926	749	860
714	401	300	419	458	303	424	390	428	389	381
345	272	307	440	451	455	280	288	279	278	292
342	310	305	277	284	319	380	324	383	288	274
345	355	196	258	248	287	403	515	208	250	178
326	332	318	284	354	293	244	324	366	225	293
317	257	347	369	223	317	311	296	369	161	335
222	449	241	219	277	213	257	241	315	246	148
319	149	376	229	289	254	279	393	400	425	137
296	294	300	328	299	435	289	373	369	441	500
335	328	356	303	350	233	618	284	400	277	347
224	363	365	324	397	666	269	310	326	304	450
286	439	420	299	238	287	432	311	416	257	407
224	446	199	433	290	367	445	205	442	299	474
418	377	235	393	467	344	301	315	244	381	413
577	563	253	414	413	370	195	323	352	350	334
224	340	362	313	401	572	710	965	408	894	351
811	666	407	351	358	903	441	444	278	395	624
388	746	765	362	415	225	454	286	453	455	430
457	640	451	494	392	525	351	437	422	337	



371

2331.8_1344EC18	264	253	229	260	267	220	253	508	401	204
203	242	285	297	295	339	211	266	293	302	280
330	219	349	244	272	345	287	258	370	322	369
361	371	351	338	464	274	440	278	259	280	261
243	269	324	251	182	325	271	251	218	272	317
263	388	438	425	241	257	424	497	469	503	310
497	458	339	310	510	556	249	305	307	627	235
758	329	218	374	293	342	240	308	302	349	412
414	408	417	203	420	203	463	432	464	430	406
449	457	448	259	443	254	449	204	243	441	442
267	453	457	471	230	338	251	322	254	313	365
311	232	212	349	361	285	313	220	240	360	441
285	289	172	218	255	246	224	289	203	205	189
315	283	958	696	958	952	999	960	940	733	854
719	406	299	419	452	323	400	373	432	366	416
294	259	264	413	436	444	286	268	156	265	272
292	294	267	265	293	293	343	257	367	285	294
325	357	204	239	227	253	420	535	199	235	155
293	347	330	261	328	297	251	339	363	236	290
295	265	317	353	253	336	291	273	379	95	346
240	456	214	213	271	147	245	202	312	261	133
308	160	353	190	268	228	279	351	404	429	101
298	266	290	320	218	438	289	361	353	469	530
307	317	359	263	324	207	638	253	413	259	388
184	341	377	309	390	667	232	274	292	291	456
271	440	438	283	207	243	442	302	417	230	412
211	442	181	436	259	357	456	182	459	292	469
432	380	190	404	458	311	277	288	226	395	414
568	574	248	407	426	401	207	320	374	319	321
159	310	360	293	411	601	674	946	411	931	355
795	664	430	340	349	932	414	426	263	397	621
362	770	768	367	403	209	429	275	441	446	439
451	648	402	442	380	492	337	402	382	308	

372

2348.0_1344EC17	287	296	227	276	291	259	274	554	438	232
229	248	321	334	317	346	227	302	300	303	301
377	247	394	271	287	380	333	290	391	352	385
376	384	404	362	495	290	500	320	269	313	293
285	306	399	282	221	344	319	303	254	294	384
276	447	494	484	280	306	481	540	512	562	349
554	481	393	349	576	592	266	353	347	654	287
766	344	258	421	339	402	281	323	344	388	437
445	454	452	242	439	242	465	470	459	477	438
496	450	459	309	461	266	464	213	279	496	498
372	471	477	485	271	359	297	337	320	330	440
348	225	228	405	433	350	387	214	328	410	458
350	337	246	258	280	289	266	320	227	219	237
391	296	938	737	957	937	960	999	926	785	869
751	451	341	461	490	391	456	435	471	419	459
377	288	308	482	491	497	317	331	255	284	335
361	343	313	302	314	328	411	308	422	299	327
359	388	229	265	274	274	457	574	218	259	179
316	353	384	297	355	320	268	373	412	329	316
299	277	319	379	272	338	333	323	421	98	363
249	524	239	259	284	163	284	268	381	300	164
363	172	422	229	312	277	316	377	466	479	136
346	274	343	374	295	508	316	403	387	495	551
389	337	380	318	372	254	676	284	432	317	444
222	422	444	352	431	666	259	371	361	291	522
301	469	480	317	249	275	481	348	457	265	474
231	451	217	450	305	405	466	240	469	329	527
456	447	225	430	506	367	310	352	245	426	450
640	631	269	440	437	434	257	382	423	388	367
194	374	407	371	443	654	695	924	453	934	392
812	677	475	384	388	945	484	511	307	467	701
431	785	777	410	477	231	486	288	498	494	474
487	669	481	530	445	570	362	470	449	366	

373

2350.9_2011EC22	276	302	220	277	282	254	260	493	393	221
223	247	319	331	306	324	215	309	290	315	265
322	221	353	266	253	322	315	277	366	334	361
345	350	343	345	438	237	442	298	259	319	265
286	318	397	282	200	336	323	295	267	321	362
261	398	423	410	256	284	407	509	453	521	323
525	443	338	321	546	535	290	310	333	607	255
705	324	273	383	335	368	290	342	313	364	407
406	417	419	283	401	232	441	425	451	421	399
440	440	450	230	443	222	452	237	280	447	449
402	440	444	448	259	380	261	323	322	312	399
372	285	210	368	396	351	417	235	308	381	432
367	322	241	257	294	311	205	305	246	248	198
426	295	926	665	923	926	940	926	999	777	833
730	429	341	438	467	328	438	405	455	409	451
321	240	270	458	471	468	334	295	273	256	300
352	301	286	279	278	318	385	326	409	269	306
313	362	194	265	278	260	412	506	195	257	163
316	330	359	263	337	332	231	335	374	281	289
326	259	315	374	270	333	327	307	343	52	357
277	471	211	236	274	163	283	248	378	284	153
343	181	408	232	331	282	288	394	424	438	79
336	354	332	353	299	469	273	383	367	441	517
303	341	355	287	357	283	643	263	392	277	394
256	386	417	345	382	647	296	315	361	189	467
294	432	444	286	278	251	450	317	420	285	406
148	450	245	470	311	368	428	204	430	321	485
427	415	248	395	489	350	339	333	273	393	421
583	556	290	428	436	419	267	379	385	362	343
163	321	406	370	428	597	725	914	398	894	356
782	675	432	350	370	917	482	448	277	439	655
395	756	739	385	428	232	453	225	464	471	435
516	664	461	530	422	575	328	439	449	364	

374

2383.0_2011EC24	318	336	209	343	347	309	328	450	471	267
323	291	327	360	377	370	314	353	310	351	315
383	256	414	320	301	374	357	342	396	349	385
392	387	422	467	508	269	477	360	319	329	352
329	352	421	301	227	396	359	332	338	318	418
304	430	449	446	318	305	445	572	461	535	420
530	464	415	420	534	534	308	407	412	608	316
665	404	306	461	397	536	349	370	483	451	425
434	440	450	291	448	265	452	461	447	470	432
471	443	424	269	431	263	425	294	295	466	459
442	471	462	453	335	438	234	421	382	421	467
433	272	277	450	456	436	406	280	378	444	475
417	392	351	352	313	272	251	332	320	263	224
443	264	746	697	744	749	733	785	777	999	758
727	436	454	451	462	435	466	426	448	493	448
444	256	311	481	463	460	353	402	304	400	428
349	324	399	375	298	292	475	381	446	268	336
401	407	255	259	289	328	478	433	197	319	169
303	333	396	297	380	332	296	412	426	283	306
312	238	299	353	287	422	330	356	399	245	437
241	518	173	240	308	145	354	264	399	309	215
357	139	447	304	342	313	319	407	463	450	137
351	380	353	391	334	490	291	368	430	484	503
371	353	373	329	379	275	615	317	412	343	403
190	465	469	363	407	614	299	418	397	227	537
307	448	443	290	270	263	449	353	441	271	459
230	431	263	456	317	401	460	271	480	346	468
438	490	295	441	485	390	320	321	311	454	469
580	485	321	484	439	476	230	424	450	424	375
221	341	423	449	451	632	686	742	431	742	393
710	687	445	508	487	812	500	486	322	450	710
468	698	635	402	469	217	484	278	476	456	433
538	669	536	576	475	622	389	515	482	398	

375

2440.4_2011EC32	276	246	230	252	242	235	284	500	358	249
217	253	279	302	339	361	270	309	353	301	251
355	253	364	253	279	387	337	253	354	279	350
339	337	330	349	449	282	440	310	267	286	265
254	294	397	244	219	338	276	246	214	282	397
236	392	418	408	247	282	406	510	465	511	301
507	432	314	308	509	551	244	313	318	654	267
789	339	283	371	328	414	259	351	346	346	370
377	312	398	185	393	236	382	432	381	466	334
467	358	361	305	378	291	364	227	278	496	495
316	431	435	436	229	411	178	324	305	327	452
385	210	212	433	468	430	352	256	269	381	454
313	306	269	234	263	217	277	294	188	226	260
365	237	848	737	847	860	854	869	833	758	999
756	430	322	407	447	310	414	432	450	424	412
320	267	305	408	442	437	287	288	249	299	292
365	327	317	283	292	310	365	366	412	293	261
386	337	174	251	241	284	371	513	190	262	144
286	355	355	306	379	323	240	375	369	292	314
292	232	286	301	229	356	304	304	380	189	367
172	436	226	298	255	170	241	283	419	258	205
363	152	367	180	270	260	254	358	374	406	180
293	302	303	370	295	439	241	354	347	444	534
308	342	336	252	270	210	694	240	439	291	421
207	332	405	302	418	720	242	336	292	234	460
278	460	392	290	227	296	413	276	412	248	424
229	374	177	381	293	364	427	205	434	296	482
426	452	233	420	500	327	231	320	268	405	464
579	586	270	426	392	383	221	324	371	342	347
198	338	324	334	448	633	658	853	432	837	363
847	713	469	325	336	875	449	462	267	448	726
426	774	746	352	436	180	438	275	450	455	438
498	697	399	453	419	466	305	396	375	339	

376

2474.0_1344EC24	252	267	230	289	276	229	278	529	430	230
230	256	264	288	361	355	258	350	408	314	292
326	236	358	213	309	316	253	253	360	303	386
360	358	327	425	502	290	489	273	246	282	311
238	276	325	248	215	314	343	215	246	250	349
273	413	461	458	230	238	457	513	486	482	284
484	458	303	288	498	572	206	308	316	582	262
665	354	224	402	324	434	230	343	444	420	465
473	433	445	265	482	219	439	449	446	485	445
485	438	406	277	411	283	410	183	212	492	493
264	474	479	502	252	327	224	360	265	360	375
307	214	206	421	377	307	271	190	274	326	600
315	274	265	250	278	135	300	281	234	192	217
285	193	707	724	719	714	719	751	730	727	756
999	399	365	449	477	373	423	446	445	432	425
372	343	267	448	436	449	283	386	277	340	387
313	327	339	362	319	283	350	321	405	360	302
339	400	142	200	227	278	431	530	192	258	121
280	393	339	267	421	347	330	351	337	262	251
297	184	254	286	233	396	292	280	377	218	416
160	492	215	248	231	146	245	199	347	276	174
402	101	344	221	248	275	317	333	469	448	195
291	274	255	334	261	506	210	353	410	503	528
256	350	296	285	334	181	603	239	486	302	382
162	368	390	377	459	581	177	298	274	239	501
307	519	377	291	172	305	465	318	402	243	396
277	447	184	455	269	416	494	214	497	316	454
499	414	206	457	530	285	197	314	231	459	627
592	667	247	464	454	397	190	364	417	292	265
210	313	412	423	435	687	500	722	428	700	363
719	931	483	370	375	755	430	477	321	442	731
443	745	654	390	481	181	431	236	459	466	533
511	700	378	400	379	447	365	384	330	323	

377

2640.8_1194EK21	257	260	106	296	281	263	266	210	499	232
238	285	271	293	330	400	245	362	361	288	298
365	242	427	236	251	357	287	290	404	340	411
386	379	330	390	624	164	553	315	255	260	313
233	300	433	277	192	290	265	208	280	279	443
288	539	524	543	238	260	519	296	646	231	349
256	604	370	356	227	371	252	366	321	339	262
277	349	220	424	288	429	167	379	381	461	579
580	495	554	247	553	179	519	500	516	630	483
630	506	493	159	517	165	500	167	209	596	598
271	551	564	617	291	418	180	395	248	406	457
406	269	209	515	488	367	241	202	263	387	496
299	306	201	252	279	143	165	276	258	218	208
262	176	380	421	398	401	406	451	429	436	430
399	999	459	777	770	452	848	891	765	842	710
445	189	320	801	826	829	227	303	208	291	305
273	359	276	288	216	216	326	337	913	214	310
363	318	109	186	258	266	516	221	173	297	134
270	413	394	242	431	305	323	367	383	281	243
243	146	242	334	254	318	340	262	354	198	383
193	572	214	255	273	13	237	215	426	281	172
377	0	355	252	312	225	300	323	498	547	94
245	136	292	389	279	588	211	375	468	653	492
293	343	285	259	354	209	344	151	558	311	511
142	414	548	442	471	220	189	417	192	225	538
329	548	481	290	163	277	605	363	565	132	504
317	469	182	509	224	452	582	186	585	349	774
506	505	176	484	388	246	190	324	252	478	544
395	198	277	512	523	513	260	448	481	276	261
190	325	466	391	526	497	268	391	547	436	446
417	334	643	459	411	452	443	892	349	480	423
887	533	209	674	862	177	735	214	835	828	580
371	603	324	371	361	336	213	349	254	346	

378

2660.0_1135EC00	260	216	114	300	317	219	255	196	400	181
	252	196	239	336	359	304	255	409	370	234
	303	220	307	230	248	373	264	220	399	292
	392	380	325	407	458	256	410	334	245	298
	266	311	418	223	231	353	342	180	261	256
	248	410	392	394	305	312	378	312	428	172
	298	407	347	299	201	340	234	334	345	308
	268	288	243	384	241	392	185	296	331	431
	406	414	425	286	428	170	342	417	341	518
	524	312	346	186	363	197	359	139	264	505
	298	359	367	403	234	304	154	328	216	332
	312	194	170	450	410	299	230	219	245	377
	256	229	264	206	241	249	158	304	223	250
	285	221	255	372	282	300	299	341	341	454
	365	459	999	441	449	482	423	380	460	425
	669	187	279	417	400	404	173	315	185	332
	264	284	310	313	226	231	306	289	426	205
	305	351	103	199	210	255	386	166	176	235
	279	358	304	288	412	285	140	340	326	283
	296	155	233	312	209	307	347	229	347	125
	164	486	241	285	259	30	277	275	338	265
	299	304	376	245	286	348	262	274	425	440
	240	88	349	384	237	449	154	388	428	470
	267	374	241	252	312	252	377	179	407	322
	172	335	379	352	313	223	190	282	206	124
	234	394	340	286	199	233	451	269	436	270
	16	329	188	350	266	405	394	185	401	322
	365	370	219	397	318	224	158	279	221	376
	362	194	252	371	379	385	242	376	395	239
	182	277	354	358	404	385	227	293	494	327
	284	332	566	372	367	328	411	460	508	447
	389	326	192	278	428	198	372	162	423	395
	373	364	262	333	265	290	205	281	263	260



379

2693.9_1344EC76	295	307	170	323	310	273	319	248	555	281
286	377	304	331	351	424	279	367	342	369	435
447	247	453	259	282	455	342	297	525	371	489
534	519	421	434	679	205	600	367	373	303	318
258	324	507	338	197	348	354	222	300	290	497
348	573	572	587	269	347	565	308	653	268	505
297	657	508	510	265	385	248	534	331	333	305
315	518	250	459	320	443	168	411	479	550	580
577	540	547	254	576	158	680	663	693	650	535
665	687	673	209	679	165	671	239	270	672	672
327	658	664	649	311	502	252	486	286	489	562
469	303	287	572	591	414	252	223	313	424	582
303	375	251	330	310	211	215	308	304	278	207
291	234	423	418	432	419	419	461	438	451	407
449	777	441	999	969	438	934	761	774	903	748
413	240	324	831	876	876	239	393	207	344	401
352	377	338	397	243	248	360	415	770	299	336
404	372	181	190	261	319	588	203	184	348	149
272	397	426	245	419	320	468	417	414	273	258
331	165	337	414	271	327	353	308	404	229	448
241	668	202	238	327	20	267	229	488	312	280
408	104	406	268	382	293	352	335	629	581	53
270	160	388	409	331	588	237	376	510	685	535
297	291	263	269	417	248	345	198	567	323	528
196	466	565	362	663	221	221	340	269	211	624
332	713	610	286	181	231	601	447	563	160	592
391	634	146	666	247	461	697	183	700	320	788
670	614	221	702	350	295	238	341	249	696	594
403	128	321	646	640	589	350	432	541	327	332
187	330	482	463	689	496	303	428	526	437	492
479	397	596	501	492	442	450	786	322	445	444
786	543	203	774	774	114	837	188	884	880	758
349	555	352	404	352	359	248	407	315	320	

380

2709.9_1344EC79	279	299	168	314	300	272	299	260	567	248
269	370	290	322	333	399	251	359	345	348	456
442	242	447	240	270	452	332	298	516	376	492
517	503	408	422	695	197	607	367	364	301	314
238	311	509	341	190	341	347	215	299	282	493
347	584	581	597	264	338	574	313	669	280	508
306	676	510	514	275	391	240	536	328	351	289
331	546	244	473	287	446	169	395	486	546	583
579	549	557	240	584	161	668	691	682	664	542
679	671	663	193	665	171	657	229	268	683	683
325	673	679	663	310	500	254	485	292	490	564
460	288	278	584	602	414	266	211	311	419	573
307	368	254	324	296	215	206	291	314	283	206
299	222	448	438	459	458	452	490	467	462	447
477	770	449	969	999	444	919	754	804	914	753
428	242	314	834	860	867	238	411	143	366	418
371	412	359	395	226	266	357	415	765	268	323
394	376	188	184	261	299	606	232	149	331	139
264	386	432	250	422	296	491	414	416	286	248
314	160	318	397	273	306	342	293	395	249	451
192	680	202	211	316	139	251	225	485	309	268
423	104	407	268	387	294	350	326	658	587	45
262	177	370	406	314	599	236	368	513	705	556
294	298	297	262	425	235	369	177	565	323	526
155	476	584	358	677	219	220	378	276	200	627
318	731	609	280	176	239	605	489	573	177	593
430	627	148	665	243	441	716	169	719	322	788
699	624	207	713	346	294	245	337	271	704	596
418	122	320	649	642	601	364	456	532	322	320
185	327	492	460	720	532	316	446	523	460	493
525	417	615	498	483	478	454	794	339	425	456
780	555	226	751	774	122	842	182	869	870	782
365	564	348	409	345	363	237	409	324	308	

381

2727.0_1344EC26	265	278	220	279	271	250	241	218	418	251
234	241	273	352	323	381	232	422	299	326	243
313	261	392	251	244	323	331	301	353	351	357
350	345	319	387	462	251	474	314	232	285	339
249	289	392	275	180	302	351	281	226	262	399
335	413	404	393	229	304	389	277	443	233	252
271	418	309	263	219	379	233	272	293	334	295
315	340	231	405	353	425	338	339	328	413	384
393	394	407	220	416	364	366	407	368	494	396
490	353	357	271	380	357	386	235	226	516	508
335	382	388	427	303	390	190	357	327	364	399
379	168	202	423	424	404	319	234	253	413	394
354	339	211	265	246	211	288	326	258	220	253
328	203	320	396	332	303	323	391	328	435	310
373	452	482	438	444	999	425	414	438	437	428
522	286	300	441	407	409	237	269	199	309	308
298	235	301	293	297	318	410	330	437	298	295
360	338	207	226	249	241	450	233	199	261	170
270	369	346	283	470	281	224	432	361	271	277
247	180	256	336	276	312	371	283	361	117	405
163	504	209	266	301	194	239	211	336	300	130
354	152	388	208	298	330	378	251	408	421	56
301	271	323	366	270	514	230	377	399	480	453
259	325	217	270	335	232	380	183	439	334	373
231	373	437	334	391	309	241	345	338	252	467
303	406	380	276	204	159	439	292	441	363	461
133	381	238	377	255	343	408	191	420	327	510
400	405	213	414	368	350	235	337	234	394	387
388	308	260	420	397	383	261	386	386	375	318
162	340	368	344	425	430	255	297	453	318	361
292	326	545	348	333	397	463	487	721	429	342
435	385	244	330	470	180	432	271	446	434	398
392	361	395	434	380	378	291	406	349	317	

382

2741.2_1344EC78	289	311	165	304	295	277	296	224	554	247
273	337	312	329	334	405	270	353	339	360	403
428	243	445	267	277	422	363	301	521	364	485
521	498	415	425	669	205	575	352	352	306	300
254	316	497	324	203	346	337	213	306	277	464
342	564	543	561	276	312	535	322	640	252	483
293	650	481	493	263	367	261	503	332	314	312
302	498	257	451	279	441	174	362	468	500	558
557	528	555	275	571	147	648	625	648	622	517
637	641	628	210	629	182	623	231	271	649	648
311	640	644	638	326	460	247	484	280	487	511
426	276	248	541	549	380	263	204	310	413	512
301	350	235	294	299	210	217	303	295	263	204
288	228	401	411	418	424	400	456	438	466	414
423	848	423	934	919	425	999	812	782	948	741
401	270	327	879	922	926	218	382	198	308	362
346	374	297	345	254	254	356	365	817	293	312
388	377	192	211	263	296	570	211	191	319	149
286	402	410	246	416	337	428	412	408	282	263
317	172	325	405	267	326	341	294	399	212	416
210	644	205	232	315	17	251	225	454	316	229
400	104	401	269	365	278	367	338	608	573	53
274	143	357	397	312	573	251	363	513	680	515
284	329	292	262	414	248	329	216	524	335	516
205	453	570	396	607	217	231	353	267	209	584
315	672	559	291	185	247	578	471	549	150	547
409	583	152	629	254	475	668	203	670	329	763
631	567	218	638	339	297	243	353	281	638	557
413	163	335	581	597	555	332	477	539	314	328
183	350	485	419	646	486	305	407	503	409	499
446	376	574	488	457	435	446	822	302	426	426
826	526	219	840	792	115	864	205	925	925	704
338	571	376	420	337	365	235	398	316	326	

383

2744.2_1288EC01	245	286	144	266	244	232	255	221	468	233
215	282	254	249	282	341	235	320	310	314	309
376	232	420	209	227	362	262	239	374	331	363
341	332	333	424	596	205	518	290	285	246	267
217	266	410	269	178	322	238	194	251	233	485
314	489	480	491	232	269	471	296	565	236	378
259	541	381	388	232	372	228	387	299	319	271
274	394	223	416	252	418	188	341	447	441	519
517	477	500	234	511	208	466	513	463	592	467
590	451	452	152	460	213	438	187	242	582	585
295	516	528	551	288	443	200	401	259	409	465
436	263	303	494	484	435	258	202	276	397	534
280	305	238	322	274	137	156	253	267	239	211
289	147	361	410	381	390	373	435	405	426	432
446	891	380	761	754	414	812	999	726	815	674
395	193	304	797	802	817	201	393	197	359	384
354	431	346	359	218	317	299	413	880	206	284
335	309	157	188	227	255	495	229	173	258	116
221	345	405	233	388	299	338	359	373	307	231
248	150	221	282	231	305	300	241	318	197	416
179	541	181	247	254	10	224	191	391	287	200
409	1	312	225	300	203	341	314	466	493	75
221	179	295	327	251	520	235	319	418	577	466
274	314	247	258	333	178	319	164	530	309	488
159	399	516	378	604	201	193	346	230	197	545
267	638	466	254	159	239	526	398	502	142	437
405	417	176	472	223	407	541	208	534	329	705
604	485	160	481	352	246	197	299	234	445	565
354	155	276	480	470	438	239	446	411	251	241
173	314	413	363	547	460	307	375	492	387	394
436	399	566	432	384	417	378	825	286	412	426
964	557	178	642	949	157	724	192	818	819	656
326	550	309	340	324	331	199	360	263	297	

384

2744.4_1135EC00	276	276	126	313	312	289	324	234	623	243
260	349	296	298	371	377	283	355	335	328	421
426	245	474	287	257	422	307	310	540	399	502
533	506	408	485	780	196	673	341	339	296	296
269	306	564	358	210	330	345	248	277	269	489
333	692	706	710	264	313	701	320	763	257	463
317	740	468	477	259	385	253	495	327	352	294
338	545	249	462	344	437	227	360	481	645	721
701	672	737	259	731	178	629	676	641	732	662
733	633	645	205	658	200	647	228	252	712	698
322	684	698	764	332	468	240	520	351	526	521
466	271	313	607	603	432	284	230	307	417	566
359	338	239	323	319	217	189	305	305	280	173
314	213	399	479	420	428	432	471	455	448	450
445	765	460	774	804	438	782	726	999	767	938
427	210	317	814	743	743	204	453	297	488	461
471	475	484	501	270	364	370	501	701	257	341
379	363	164	195	261	324	650	243	195	321	137
261	342	484	246	415	280	452	392	440	296	266
226	214	250	324	285	321	323	282	382	170	493
188	708	176	230	296	133	253	227	536	325	260
428	134	456	260	376	278	360	298	664	667	22
293	200	372	400	330	671	249	424	536	784	547
330	282	243	261	423	242	350	230	584	326	609
180	538	590	397	611	251	233	334	294	246	631
362	695	581	294	193	274	794	456	782	224	568
421	550	158	613	255	413	702	232	717	349	772
663	616	235	634	348	275	261	323	248	610	569
411	205	322	595	645	635	391	441	573	321	306
203	318	598	472	673	561	286	380	533	430	537
506	378	596	592	537	514	460	762	330	457	461
739	532	219	667	748	169	734	172	777	779	727
349	535	352	401	323	379	244	388	320	326	

385

2765.9_1344EC78	254	295	188	309	295	288	317	263	546	231
256	355	319	298	309	388	262	330	322	331	431
420	222	424	274	282	422	368	322	499	358	464
509	481	409	410	647	237	573	368	341	312	295
257	311	501	347	216	360	350	252	293	281	457
342	588	566	581	277	296	564	330	649	280	462
305	655	480	485	314	391	263	508	313	358	287
337	506	261	461	319	446	244	350	503	529	576
572	553	569	256	577	186	636	632	641	620	535
632	635	637	225	640	223	636	221	264	655	653
379	654	657	643	307	477	236	486	309	491	531
447	276	223	557	567	419	302	228	320	434	519
351	361	262	298	316	246	220	288	305	258	184
333	241	360	413	379	389	366	419	409	493	424
432	842	425	903	914	437	948	815	767	999	724
383	260	309	873	890	907	254	405	232	364	402
337	383	343	360	266	275	399	376	833	287	319
372	363	196	234	264	317	566	250	198	304	158
313	381	444	236	407	312	456	385	410	294	262
290	223	313	372	269	308	333	292	387	205	401
175	625	202	214	307	125	258	238	439	319	277
397	146	400	267	373	291	358	340	608	574	137
267	209	332	383	316	586	252	362	482	681	503
341	301	299	260	380	269	366	232	535	331	515
216	430	564	387	614	232	250	338	314	205	569
342	661	554	288	204	268	595	485	574	232	550
419	564	204	637	266	435	666	219	671	325	755
632	582	235	646	358	318	283	333	285	649	550
401	247	331	585	615	585	355	469	537	345	337
191	353	486	437	627	482	333	387	483	373	474
463	382	576	493	463	403	440	790	328	478	439
830	517	221	808	804	169	860	255	897	910	722
370	575	435	465	374	413	298	439	384	318	

386

2766.5_1135EC00	278	293	146	304	299	296	344	256	653	250
288	346	307	319	378	438	289	362	351	349	413
439	239	500	292	273	429	318	319	569	393	532
560	535	435	486	781	229	685	358	345	298	303
286	314	569	340	204	360	328	248	318	269	490
326	702	693	706	270	312	687	322	743	253	471
310	725	476	486	257	393	270	504	321	355	310
331	507	260	457	358	426	225	382	497	627	717
711	666	733	282	744	187	623	658	638	735	659
725	623	630	213	642	203	630	246	257	689	678
334	673	686	746	323	469	223	535	328	542	539
466	269	277	600	608	422	262	226	302	396	546
349	361	253	312	310	220	195	299	304	284	148
286	216	399	460	399	381	416	459	451	448	412
425	710	440	748	753	428	741	674	938	724	999
427	200	317	764	701	691	204	411	311	470	418
477	483	470	481	276	353	366	496	668	226	335
387	377	171	209	277	344	670	257	199	342	155
262	395	494	276	433	300	446	403	435	318	280
255	213	247	347	283	330	327	297	419	169	490
204	731	166	240	300	118	271	245	547	313	248
435	126	449	300	380	284	343	301	655	684	122
268	235	354	386	368	661	255	440	569	767	562
346	299	241	279	424	265	361	250	593	318	597
179	512	615	417	625	248	248	339	314	227	632
354	715	598	308	200	278	772	443	770	213	574
432	543	176	607	261	419	697	224	708	326	771
682	619	230	602	355	295	265	318	300	593	553
418	189	348	585	622	655	381	483	566	347	306
205	314	591	486	671	561	310	385	526	451	565
480	357	583	602	578	470	447	745	325	481	449
716	499	217	639	728	153	710	178	718	736	704
349	513	338	398	329	388	252	398	341	321	



387

2775.3_1344EC07	247	268	198	293	287	254	283	207	418	244
	244	266	272	378	356	367	298	456	344	267
	314	249	362	282	284	366	315	303	371	364
	370	361	338	418	492	244	471	323	263	277
	272	308	408	277	200	350	350	302	258	284
	290	432	387	384	196	292	373	295	457	211
	289	426	298	241	225	353	251	273	295	318
	267	312	252	368	275	398	316	325	350	431
	427	381	442	248	422	298	359	441	356	502
	507	339	358	290	385	248	373	191	237	494
	366	403	415	456	301	346	234	342	312	345
	317	208	229	453	430	329	401	228	185	445
	397	315	421	264	267	231	245	314	225	237
	418	215	271	359	317	345	294	377	321	444
	372	445	669	413	428	522	401	395	427	383
	999	250	279	426	382	393	268	350	191	333
	312	286	335	341	325	345	372	348	421	307
	419	339	211	211	236	283	432	243	238	297
	273	373	343	297	490	278	215	390	341	295
	261	209	289	351	298	358	369	271	360	81
	198	511	227	219	302	126	261	229	334	297
	345	261	370	237	303	354	302	278	419	454
	282	232	302	347	244	488	275	386	402	508
	260	315	276	270	311	261	355	174	458	344
	207	367	436	317	368	274	239	307	357	228
	284	405	391	291	214	253	444	289	438	330
	192	372	242	397	283	360	405	150	416	360
	379	402	226	387	341	291	243	318	207	370
	386	174	277	436	412	432	260	414	433	330
	151	306	380	332	428	376	292	245	438	296
	294	313	549	362	355	388	424	474	481	448
	415	351	229	291	455	194	376	211	398	404
	363	371	389	416	394	392	265	373	351	301

388

2800.0_1129EC05	187	216	677	160	167	111	163	154	128	143
294	94	164	160	193	166	161	247	302	262	122
145	226	27	121	288	142	185	122	167	185	49
178	137	223	157	35	764	302	96	206	195	264
211	173	0	181	118	214	187	176	186	162	153
162	227	197	205	191	142	205	161	10	131	216
174	120	240	235	150	241	189	270	369	189	231
203	284	222	250	239	302	187	210	336	207	143
172	112	147	3	122	288	248	235	273	233	122
264	242	224	891	368	222	340	330	161	312	288
0	155	96	121	215	239	91	296	199	288	335
274	138	255	107	126	87	139	182	178	221	194
190	173	290	194	187	182	952	231	455	87	265
194	163	250	252	273	272	259	288	240	256	267
343	189	187	240	242	286	270	193	210	260	200
250	999	93	245	253	261	296	192	84	253	243
117	3	157	0	942	135	295	215	259	958	144
109	209	281	142	129	163	94	60	135	36	240
114	0	205	246	223	175	0	0	116	0	133
146	148	120	122	150	273	293	144	170	155	55
142	0	177	67	114	231	174	60	28	132	196
169	106	86	228	208	156	161	110	0	201	43
184	162	159	0	87	121	157	189	1	12	266
121	16	5	404	116	206	16	97	126	224	0
106	205	10	0	169	0	188	108	230	224	214
270	0	239	150	157	161	29	12	97	59	78
0	180	69	0	161	141	92	215	67	94	210
65	251	145	79	227	312	181	243	183	122	110
133	0	53	345	126	85	95	6	128	292	284
0	251	236	148	0	247	91	66	142	86	1
138	178	273	51	252	1	265	71	0	263	226
40	167	4	120	246	103	161	237	83	3	67
247	109	312	350	195	164	210	194	167	173	

389

2834.5_1180EC112	236	158	80	284	269	318	219	151	303	
174	237	404	180	197	219	256	215	225	141	209
195	354	365	411	292	208	274	191	186	303	230
251	279	269	267	239	291	153	266	307	229	208
244	217	177	264	173	110	228	232	234	287	218
215	218	297	285	298	226	288	287	188	299	161
451	182	325	435	459	167	271	245	455	263	243
277	164	207	214	281	207	292	235	287	294	296
283	305	291	262	131	258	215	337	280	341	317
291	318	340	328	129	331	164	335	232	190	315
312	223	316	306	299	235	230	227	315	184	311
249	250	242	272	313	301	264	222	221	191	320
301	229	238	234	240	223	241	123	173	286	259
212	209	239	259	312	291	307	264	308	270	311
305	267	320	279	324	314	300	327	304	317	309
317	279	93	999	318	312	290	241	262	4	224
273	179	7	225	256	60	248	255	304	314	105
265	188	239	94	138	316	219	297	65	78	383
105	6	201	187	17	45	148	130	377	314	217
280	203	6	264	301	175	170	225	319	162	0
215	246	306	50	7	225	5	103	158	256	204
151	209	0	280	63	248	203	193	113	285	297
3	115	227	322	185	184	321	135	280	338	326
314	139	13	70	213	165	193	159	161	322	249
202	130	290	319	12	281	58	185	268	49	5
326	206	168	301	761	188	125	280	209	227	2
323	0	143	81	317	168	196	320	143	326	186
316	283	302	143	286	168	608	37	758	276	270
250	293	19	226	303	331	272	228	213	269	587
569	244	770	292	103	283	313	29	222	255	269
352	336	243	276	276	286	290	366	341	144	166
297	286	244	9	264	310	128	240	74	302	274
277	242	282	244	329	319	248	153	284	204	371

390

2836.1_1288EC38	241	238	165	300	292	233	306	217	527	249
245	328	249	279	312	368	273	350	323	336	390
383	237	423	216	249	401	284	267	441	332	414
436	412	391	427	674	223	589	321	339	230	312
208	289	528	313	185	350	317	239	264	272	469
304	561	545	561	210	311	542	287	654	251	405
261	670	408	435	230	332	215	447	318	328	278
308	482	220	474	285	457	178	340	588	537	603
591	526	603	215	583	144	597	605	613	646	517
651	599	599	203	617	196	596	217	258	664	666
308	636	653	691	289	417	242	463	282	472	516
397	274	244	575	577	398	224	243	292	407	501
297	318	243	281	235	160	207	241	300	281	233
259	161	420	461	430	440	413	482	458	481	408
448	801	417	831	834	441	879	797	814	873	764
426	245	318	999	826	834	231	433	325	410	421
383	433	375	453	244	297	344	402	825	285	313
335	348	118	196	217	306	561	201	145	293	125
209	358	413	251	389	277	449	359	363	299	234
227	151	236	284	236	305	291	259	347	273	440
175	632	179	247	295	35	230	184	485	285	243
421	0	390	243	339	258	308	303	597	578	61
260	165	348	365	246	602	195	321	468	704	518
279	294	260	253	431	183	318	245	554	293	533
199	491	587	361	657	226	204	385	199	190	573
311	706	548	279	146	262	625	514	592	180	514
444	515	177	575	231	450	682	176	690	322	751
660	594	176	633	338	258	184	324	270	626	564
371	98	316	591	603	585	346	458	534	298	257
176	331	474	454	673	521	280	431	486	396	463
517	371	576	525	480	481	407	833	299	418	451
842	553	203	720	809	180	810	207	865	868	753
332	577	304	352	319	317	251	359	275	301	

391

2872.9_1344EC15	311	303	153	312	314	297	300	243	520	278
286	336	318	313	326	410	283	352	327	366	422
436	266	429	268	270	420	363	319	495	378	449
518	498	397	403	635	187	537	355	349	293	308
262	321	473	318	211	339	349	217	317	287	450
357	571	559	571	291	323	552	332	611	269	488
299	626	513	517	280	365	267	522	332	343	325
313	510	272	461	292	451	183	378	456	452	529
529	484	519	251	530	138	601	636	599	597	474
609	594	586	200	589	191	582	233	286	605	606
343	571	585	602	326	490	278	439	280	445	499
468	301	263	517	529	408	268	224	316	449	471
311	344	229	294	313	225	213	328	305	304	199
296	237	431	441	445	451	436	491	471	463	442
436	826	400	876	860	407	922	802	743	890	701
382	253	312	826	999	971	207	373	229	340	357
355	409	332	367	246	287	352	396	823	281	316
382	344	198	211	284	300	535	222	224	321	150
288	388	401	247	405	329	443	390	411	298	277
337	178	354	431	281	321	346	322	376	210	417
223	612	201	199	318	15	263	228	438	308	251
392	0	398	261	378	285	378	350	573	567	40
251	143	367	368	324	558	243	356	485	653	534
287	320	294	256	397	250	347	196	486	322	495
212	442	539	390	626	237	249	360	249	200	571
308	663	541	277	193	243	559	500	527	135	508
411	525	154	571	259	474	606	187	610	337	743
638	540	230	637	350	290	251	331	286	640	511
429	172	303	528	523	512	297	441	473	304	309
210	329	464	401	644	501	318	442	486	451	462
490	378	542	439	432	461	437	795	283	397	414
821	561	258	825	782	111	895	219	978	964	689
336	534	365	410	345	362	239	394	329	321	

392

2906.6_1344EC15	292	302	154	308	311	292	297	238	538	236
254	347	309	299	310	379	251	341	297	363	434
434	243	426	237	254	414	350	317	493	381	460
510	488	374	400	650	194	545	348	353	303	293
231	308	490	338	208	330	333	215	292	283	450
357	593	575	588	278	326	572	318	619	253	473
294	633	510	497	263	361	248	520	322	340	293
300	513	259	483	309	472	188	385	460	472	543
537	497	530	233	536	137	599	643	607	615	484
625	602	602	194	604	179	597	219	268	627	629
349	590	603	616	322	497	284	455	288	461	504
461	286	269	526	542	403	267	207	300	439	490
317	348	217	309	304	214	207	305	309	289	198
296	225	437	453	450	455	444	497	468	460	437
449	829	404	876	867	409	926	817	743	907	691
393	261	290	834	971	999	238	369	209	346	354
354	395	345	360	248	281	357	396	834	276	314
375	348	199	187	285	297	559	200	184	305	141
283	378	419	234	396	310	437	381	402	297	259
318	166	333	403	266	307	328	298	378	211	424
186	620	196	193	315	97	234	207	425	309	263
408	0	395	254	365	269	353	335	587	576	35
260	168	361	381	332	566	235	354	466	666	529
296	296	304	252	393	242	340	170	499	315	499
172	444	536	378	614	226	248	373	248	195	583
312	673	563	271	185	248	572	509	534	125	511
424	537	156	586	252	450	621	183	628	334	748
650	558	212	636	345	266	259	324	284	633	526
417	186	271	530	546	538	334	432	475	301	286
206	324	471	409	653	515	305	441	478	449	428
515	383	551	438	428	474	445	780	281	405	421
834	564	199	819	796	103	888	190	964	986	694
344	541	363	403	344	364	236	404	336	307	

393

2911.5_1344EC10	215	197	258	193	222	242	241	303	239	214
205	214	190	239	227	157	229	212	215	249	175
260	245	222	261	190	221	206	235	230	268	227
224	219	222	170	224	295	269	222	179	249	203
202	201	229	180	182	219	184	276	196	234	189
214	212	202	225	216	220	214	288	209	284	228
262	189	258	230	281	289	200	276	217	286	223
314	263	201	239	250	281	243	191	253	202	167
218	158	181	153	197	233	207	239	218	206	207
219	206	198	259	225	276	210	231	214	223	221
292	219	221	225	206	172	226	247	324	252	257
174	219	255	232	261	207	325	154	254	266	237
315	257	227	285	230	197	303	230	209	125	154
320	195	295	288	299	280	286	317	334	353	287
283	227	173	239	238	237	218	201	204	254	204
268	296	241	231	207	238	999	128	279	250	241
188	152	212	162	277	218	412	266	227	272	193
203	211	264	209	253	241	264	305	193	215	201
183	167	190	216	211	211	190	259	259	220	266
177	165	227	251	246	240	233	235	247	95	204
117	246	166	199	216	123	193	165	225	181	126
239	253	282	155	240	200	215	174	224	176	29
222	301	218	268	232	297	235	240	203	232	246
239	172	167	256	173	218	293	210	244	223	197
210	241	291	192	245	243	191	219	257	227	244
207	236	187	285	200	128	200	198	204	253	236
140	191	257	232	206	266	215	167	228	223	224
226	275	215	237	182	270	229	292	229	237	233
278	159	181	238	193	237	175	190	229	277	285
213	305	230	224	281	276	302	287	207	250	208
212	277	236	205	205	241	338	274	199	241	256
207	217	216	199	239	175	271	318	217	211	241
242	233	363	375	354	347	342	383	360	277	

394

2990.3_1164EK03	248	241	8	170	176	234	202	263	437	149
207	296	270	296	377	386	191	313	361	306	256
333	245	396	249	424	293	299	227	334	285	354
328	320	314	405	443	53	397	251	241	231	278
171	258	379	255	246	236	253	195	207	196	447
259	392	404	393	224	250	389	276	436	252	282
258	437	316	294	276	297	224	330	251	296	238
297	320	195	298	402	375	232	267	666	389	378
377	379	393	319	378	143	360	406	358	414	386
416	332	304	181	315	161	324	160	201	451	434
313	392	398	441	242	353	158	310	414	310	390
282	204	368	443	438	375	258	198	260	304	415
388	251	220	392	206	132	166	282	210	208	228
291	152	252	318	245	288	268	331	295	402	288
386	303	315	393	411	269	382	393	453	405	411
350	192	262	433	373	369	128	999	618	731	988
657	522	744	861	205	541	348	583	374	186	199
291	356	111	190	213	202	423	271	180	303	158
282	375	334	363	377	307	272	362	377	320	233
248	203	227	298	213	390	257	185	367	174	404
65	450	230	186	316	26	170	190	337	266	207
395	7	333	193	231	211	265	193	453	419	1
295	191	244	317	282	426	258	296	375	446	365
225	412	288	212	306	194	320	205	353	250	400
239	390	336	311	413	356	130	346	264	243	424
246	466	322	259	196	225	432	329	428	192	330
270	367	172	332	202	379	431	223	424	295	381
448	427	188	364	273	245	161	272	234	371	441
294	262	283	339	327	382	288	383	477	248	195
209	270	399	299	359	315	221	264	332	277	372
304	344	353	402	315	278	424	410	307	352	366
411	324	219	360	404	161	377	178	395	371	384
223	343	327	356	327	341	357	341	317	345	



395

3007.7_1164EK03	167	182	81	185	214	32	48	179	172	98
155	106	106	80	124	167	90	147	135	171	16
132	122	175	130	103	88	134	99	104	82	125
104	106	172	321	211	0	189	86	36	98	160
160	102	110	71	7	181	129	78	206	135	228
74	274	288	292	82	86	284	206	309	106	203
186	289	200	211	110	203	114	190	217	197	185
152	219	145	153	220	234	50	292	489	301	255
256	271	312	131	251	155	190	218	240	181	257
167	193	208	52	212	105	176	222	145	228	224
229	275	279	291	73	246	37	258	197	257	155
220	69	295	259	256	263	117	86	164	201	293
193	108	243	293	151	76	63	86	235	178	129
172	56	185	274	221	279	156	255	273	304	249
277	208	185	207	143	199	198	197	297	232	311
191	84	4	325	229	209	279	618	999	461	623
475	451	453	741	105	421	219	486	236	87	242
164	251	93	53	30	48	178	232	147	132	1
119	185	159	245	192	224	158	139	124	9	137
221	235	120	112	30	190	109	4	168	94	280
2	207	0	192	110	0	158	73	105	79	72
184	0	177	164	91	125	80	27	137	229	170
152	104	98	213	201	308	247	98	147	300	193
141	125	170	155	174	65	136	267	141	226	142
187	283	247	14	176	144	21	155	86	200	152
214	216	135	35	41	80	331	201	330	139	64
247	174	3	164	110	129	278	190	290	103	158
215	127	169	150	109	174	78	168	187	92	312
18	163	199	219	105	232	129	205	252	143	125
159	148	237	199	162	190	221	116	191	192	193
135	265	186	317	261	188	192	172	138	88	220
158	237	84	183	245	0	157	186	189	169	159
116	92	140	207	162	170	159	146	83	100	

396

3009.1_1164EK03	255	246	22	128	157	234	229	240	401	154
132	296	242	318	364	314	226	313	299	303	255
345	258	394	259	416	287	239	236	352	291	353
349	337	303	474	456	0	410	230	239	231	153
152	254	389	255	242	233	262	253	182	234	435
269	481	477	467	220	264	461	309	478	269	244
286	443	296	249	277	324	214	269	259	298	200
303	359	178	313	438	362	243	221	379	415	439
433	411	503	263	425	135	342	384	366	433	431
434	330	303	246	318	204	325	158	186	447	435
423	427	440	520	249	316	184	350	517	348	381
285	193	432	459	429	382	316	203	238	318	440
457	246	256	429	236	160	206	302	212	219	157
329	167	275	298	255	278	265	284	256	400	299
340	291	332	344	366	309	308	359	488	364	470
333	253	224	410	340	346	250	731	461	999	732
767	716	986	827	275	648	358	688	377	169	178
287	317	128	210	212	229	405	267	227	299	153
250	350	327	323	390	295	272	397	421	328	259
242	202	263	303	224	375	319	184	370	121	437
100	422	241	183	337	65	149	183	378	261	231
389	20	337	171	237	207	271	199	399	461	236
222	211	258	350	212	500	209	304	368	498	355
291	315	274	218	357	220	319	135	404	256	417
174	413	375	304	379	309	190	325	269	170	398
258	442	290	231	190	190	537	296	524	132	330
220	335	195	354	163	322	462	253	451	290	386
407	427	208	336	326	219	183	238	192	333	466
320	225	255	344	343	315	216	369	386	230	209
188	235	362	303	332	306	265	272	348	274	349
290	316	403	366	330	270	397	435	263	349	317
402	307	227	356	420	188	331	193	358	353	375
285	340	338	349	344	330	304	380	348	294	

397

3113.7_1164EK03	252	238	76	208	213	261	229	266	452	161
190	290	304	303	372	368	204	345	320	312	262
345	250	410	261	426	306	309	234	356	298	377
350	338	305	418	454	141	420	256	252	237	266
181	277	387	258	248	233	267	218	217	234	456
270	406	414	406	229	259	402	287	448	259	294
260	448	321	306	271	301	235	335	256	285	244
284	338	230	320	407	385	257	270	671	402	383
383	397	399	291	378	238	369	398	361	425	399
426	338	311	204	335	217	333	207	219	464	449
340	394	402	450	253	389	141	308	434	307	402
329	195	373	450	447	394	288	274	266	302	435
405	276	215	395	253	177	221	268	210	218	276
312	173	254	321	249	292	272	335	300	428	292
387	305	337	401	418	308	362	384	461	402	418
351	243	273	421	357	354	241	988	623	732	999
663	542	742	856	211	545	367	612	382	227	225
317	314	164	255	237	229	437	273	202	296	153
290	362	353	388	418	312	295	359	393	326	277
249	258	246	293	223	382	247	257	368	160	423
90	461	243	224	327	53	160	191	346	261	199
401	133	341	199	255	224	276	191	462	423	128
312	222	256	335	295	432	254	306	371	463	378
313	390	281	280	309	211	311	273	356	264	405
270	403	346	306	418	318	195	345	294	224	439
236	481	362	283	219	226	436	334	431	215	346
279	371	199	354	225	367	435	236	428	320	394
457	432	248	370	351	269	203	329	244	377	465
305	258	331	356	333	396	288	390	476	279	251
195	314	401	297	383	316	257	267	335	281	378
312	344	363	401	331	282	415	435	320	377	369
414	323	214	364	399	185	368	205	385	383	392
277	339	338	388	358	370	368	371	358	359	

398

3138.7_1164EK03	228	213	23	204	289	131	239	242	311	124
16	262	292	251	303	293	188	266	273	301	228
310	225	368	157	313	282	290	320	301	290	338
309	321	262	420	399	4	387	172	154	184	119
198	260	341	248	57	304	280	184	267	237	401
277	451	465	452	213	215	447	300	422	279	257
310	402	310	264	276	361	237	316	238	376	257
321	309	97	313	410	382	197	280	324	446	381
372	407	454	275	347	186	341	369	379	388	413
396	324	293	149	294	184	314	171	210	429	425
340	385	376	427	245	358	147	307	443	307	406
292	160	490	444	410	355	223	218	287	283	393
394	156	138	466	261	87	118	308	172	139	146
268	150	315	341	362	342	292	361	352	349	365
313	273	264	352	371	298	346	354	471	337	477
312	117	179	383	355	354	188	657	475	767	663
999	685	803	660	148	824	258	725	328	121	309
300	271	204	125	121	239	350	256	224	301	9
296	325	347	316	305	308	226	321	388	314	139
241	4	275	305	157	264	186	243	311	9	406
84	379	190	234	338	66	201	175	324	261	30
412	5	333	190	237	176	273	162	379	425	0
148	239	201	266	246	422	230	310	365	429	355
197	359	246	219	337	197	384	1	326	222	392
24	421	374	257	412	359	59	271	170	229	380
263	446	282	213	136	182	496	319	471	161	230
326	372	173	313	191	318	405	197	443	268	352
417	403	220	298	221	169	141	155	143	303	416
319	316	218	309	334	345	264	389	411	215	119
169	171	374	305	269	300	212	301	381	309	339
303	288	367	399	331	346	372	369	277	350	288
398	365	264	354	383	136	316	14	366	367	381
247	293	257	250	224	259	210	238	193	287	

399

3152.5_1164EK03	232	177	41	44	159	38	113	107	341	23
154	194	232	248	290	375	22	215	340	282	252
124	145	285	114	252	298	252	223	274	204	241
266	252	243	396	419	0	394	61	58	129	29
220	250	337	139	11	232	278	128	265	176	357
166	416	417	400	108	246	398	213	410	81	332
211	393	325	350	23	255	171	330	289	315	249
193	397	162	337	352	387	93	207	400	335	369
374	335	440	220	360	89	309	375	364	368	349
370	311	314	3	323	44	333	251	211	440	461
245	399	411	472	232	315	35	292	282	291	356
291	205	279	387	381	314	57	158	168	237	407
246	118	282	309	136	133	16	120	257	203	34
140	111	294	297	297	310	294	343	301	324	327
327	359	284	377	412	235	374	431	475	383	483
286	3	7	433	409	395	152	522	451	716	542
685	999	697	645	3	554	199	626	379	3	209
331	293	43	243	33	113	336	144	16	227	11
250	363	302	196	280	212	356	246	259	261	4
254	0	209	273	47	300	150	22	339	5	353
2	370	0	248	304	0	223	217	246	132	17
336	2	321	157	152	140	175	235	395	394	0
3	69	220	249	210	381	3	193	343	432	341
141	360	214	60	235	135	316	0	350	193	272
4	415	400	254	441	261	93	336	161	1	357
240	510	278	14	68	191	464	283	449	63	106
296	228	6	271	107	349	445	75	450	264	343
469	380	181	332	344	9	106	8	133	331	424
97	169	283	305	284	355	199	413	389	16	3
218	14	326	201	370	297	281	286	335	321	337
328	303	349	374	352	304	213	367	187	336	322
419	311	114	303	446	3	304	0	391	389	482
269	293	78	110	14	134	161	109	142	56	

400

3168.3_1164EK03	243	246	69	156	255	232	178	243	402	126
186	260	259	296	339	314	167	327	303	305	239
330	267	379	266	402	298	269	222	320	280	319
316	309	292	455	448	128	409	219	190	215	192
185	264	357	258	188	250	217	233	186	229	412
260	433	440	427	206	275	424	248	479	260	231
245	450	286	237	266	324	209	263	251	297	217
323	328	163	303	424	358	238	211	410	423	404
400	398	473	293	404	218	335	357	354	403	413
404	319	292	161	310	189	314	170	189	434	424
355	422	434	511	231	315	140	324	490	324	379
292	141	413	441	418	350	286	199	247	294	425
434	257	194	429	212	159	139	279	182	160	238
303	176	258	310	293	305	267	313	286	399	317
339	276	310	338	359	301	297	346	484	343	470
335	157	225	375	332	345	212	744	453	986	742
803	697	999	807	226	661	382	702	348	142	210
282	288	174	225	207	178	404	271	189	258	167
273	299	327	334	405	321	274	358	396	322	245
245	249	231	304	214	318	312	211	342	94	444
112	415	247	190	296	58	160	181	331	270	154
360	138	347	174	237	189	260	136	376	430	203
291	189	253	312	262	477	247	307	361	497	341
280	327	291	250	331	204	323	144	358	241	398
153	429	340	325	363	336	180	321	269	186	392
237	422	300	232	189	211	500	296	494	235	288
209	324	190	328	168	325	454	199	443	283	357
384	413	190	320	327	255	198	270	171	307	446
285	187	266	361	303	301	208	362	361	248	218
171	273	378	303	326	291	252	264	322	270	322
274	300	364	351	299	303	376	400	255	347	297
388	328	173	326	401	191	324	211	349	353	339
296	313	345	369	366	351	347	353	329	308	

401

3190.0_1164EK03	241	201	0	169	170	221	180	236	442	124
240	302	283	294	401	310	187	264	369	300	261
321	224	406	254	390	278	285	228	347	295	377
339	329	267	440	485	0	418	240	248	248	257
167	251	376	242	221	186	268	211	219	245	442
245	478	481	470	192	231	467	299	509	240	300
274	497	307	314	239	292	253	319	278	299	208
282	356	178	302	419	341	171	264	564	415	449
439	437	525	269	448	130	371	400	393	436	451
437	339	310	0	323	116	332	199	154	457	454
337	434	445	533	253	328	150	318	427	318	379
296	152	458	461	443	364	257	227	226	274	454
404	227	262	462	240	160	0	280	195	187	112
288	142	261	305	272	277	265	302	279	375	283
362	288	313	397	395	293	345	359	501	360	481
341	0	256	453	367	360	162	861	741	827	856
660	645	807	999	0	550	324	644	342	0	198
307	292	53	208	207	180	438	269	185	308	177
285	349	333	321	345	315	292	364	368	309	244
239	118	222	290	229	348	263	190	329	227	455
84	460	235	221	330	56	166	208	351	241	189
395	5	323	198	203	199	256	252	454	470	156
190	113	200	324	209	471	141	311	372	527	319
271	391	267	174	311	185	316	258	372	203	416
230	376	331	317	404	360	149	320	251	132	429
209	472	336	293	156	305	524	313	513	135	353
263	348	144	348	172	316	483	216	493	319	381
447	435	185	353	335	210	147	281	242	354	492
313	246	284	345	345	362	267	358	478	218	235
198	251	362	295	368	315	177	279	311	296	385
266	358	384	393	350	304	367	414	284	375	292
393	306	261	364	397	148	327	107	367	359	383
255	302	245	291	267	298	285	338	305	287	

402

3200.0_1135EC03	192	266	621	176	178	97	182	142	143	179
303	91	150	170	195	185	176	230	269	306	135
153	262	46	117	295	166	180	128	171	169	49
182	144	239	194	78	674	333	89	196	184	249
230	173	0	173	20	299	206	156	232	180	200
159	228	201	208	174	155	210	260	9	210	216
266	135	265	235	215	303	197	276	358	238	272
231	296	249	248	213	332	181	194	329	197	152
197	119	157	7	132	297	258	243	282	224	147
265	262	235	869	361	195	335	371	196	304	290
54	151	91	113	232	197	129	331	209	323	344
221	183	208	109	110	101	162	161	160	271	204
181	180	338	186	160	187	890	106	431	74	272
201	188	284	275	287	284	293	314	278	298	292
319	216	226	243	226	297	254	218	270	266	276
325	942	60	244	246	248	277	205	105	275	211
148	3	226	0	999	203	305	247	258	967	141
170	243	310	166	119	182	101	93	140	39	211
110	142	243	205	199	176	0	0	105	0	123
116	144	88	83	111	307	313	162	138	173	62
20	0	149	54	116	3	208	53	28	165	8
136	107	72	157	208	184	139	175	0	196	42
190	149	154	0	53	153	188	217	1	10	315
157	93	6	429	48	183	142	122	76	242	0
95	249	17	0	231	79	206	56	213	221	224
305	0	198	164	181	236	43	76	111	58	122
0	197	126	213	163	97	79	218	58	97	234
2	252	192	78	197	307	175	260	189	103	82
144	0	1	359	100	114	111	4	178	291	276
102	260	253	123	0	246	109	114	117	113	1
12	186	295	112	284	40	274	68	1	222	203
41	238	5	106	247	97	161	177	88	30	39
278	60	373	389	237	177	102	226	149	132	



403

3296.6_1164EK03	202	157	53	177	175	171	201	169	220	220
217	219	217	214	190	221	202	242	83	273	107
335	220	371	174	190	232	217	242	189	226	190
189	187	153	234	291	65	300	212	204	219	196
182	263	250	182	116	221	229	114	223	193	323
221	318	309	313	197	168	311	259	308	223	270
257	307	293	266	162	287	205	287	170	292	198
273	187	164	251	328	308	118	280	256	338	300
317	324	362	129	307	154	187	228	278	276	319
278	198	162	169	226	142	205	205	213	320	320
298	268	263	312	200	298	154	206	414	207	304
284	173	475	304	289	303	231	208	215	281	348
353	183	188	454	263	115	161	281	279	211	191
232	183	300	284	320	319	293	328	318	292	310
283	216	231	248	266	318	254	317	364	275	353
345	135	248	297	287	281	218	541	421	648	545
824	554	661	550	203	999	285	697	296	149	183
182	26	255	272	237	201	247	145	178	271	92
150	341	256	200	238	254	11	234	359	194	198
127	136	163	226	256	84	201	245	160	146	267
225	269	187	148	218	35	98	200	245	205	60
231	1	192	179	212	197	233	198	227	316	88
213	237	187	148	188	331	215	269	195	338	299
263	213	137	235	163	177	280	180	251	197	232
96	330	322	157	339	187	195	166	166	240	299
150	322	244	197	166	109	406	229	337	130	220
337	184	180	170	199	185	292	198	314	227	293
335	275	177	203	176	237	89	217	74	202	362
258	248	253	284	170	192	170	233	268	255	202
188	212	277	156	248	261	168	232	303	263	184
219	234	320	248	218	260	322	338	205	259	248
325	326	232	176	374	90	239	65	277	268	322
189	231	289	300	299	245	137	274	180	323	

404

3374.5_2014EC05	261	364	237	287	307	251	240	265	312	224
323	255	266	313	306	287	245	288	249	352	275
341	296	311	265	304	321	298	306	326	348	254
314	283	308	313	342	275	357	288	283	312	330
249	320	242	263	252	392	321	347	337	245	305
358	359	337	338	327	316	341	370	309	323	303
357	312	353	304	320	381	292	314	404	316	338
289	351	291	309	371	446	312	312	374	404	324
321	332	319	226	304	268	330	352	329	418	335
411	322	312	279	344	346	346	336	294	421	434
319	311	312	318	318	326	262	402	371	406	320
332	297	296	324	315	286	347	322	368	389	357
376	321	288	335	341	301	298	285	364	286	312
379	248	342	391	355	380	343	411	385	475	365
350	326	306	360	357	410	356	299	370	399	366
372	295	255	344	352	357	412	348	219	358	367
258	199	382	324	305	285	999	374	363	310	290
269	304	338	212	244	240	299	227	149	253	195
217	258	297	209	311	231	247	329	334	210	253
234	182	266	313	275	328	326	347	281	156	308
222	363	191	160	288	96	241	262	254	240	229
338	114	343	279	351	270	309	356	245	322	100
291	215	326	286	295	373	248	371	267	329	420
340	162	287	319	281	302	269	240	323	312	257
211	468	315	300	286	213	281	255	346	199	383
321	285	348	334	253	203	338	224	293	236	370
209	299	194	312	282	334	298	181	313	292	393
278	327	327	312	297	423	301	362	296	275	341
265	168	213	416	323	333	176	289	360	466	380
294	382	352	366	278	327	242	310	330	354	292
276	296	371	366	401	342	516	355	244	319	350
265	377	189	264	352	141	270	403	342	284	293
400	289	482	555	474	544	510	596	578	366	

405

3397.0_1164EK03	253	223	113	164	213	257	213	303	432	163
146	301	260	313	309	349	192	297	323	287	227
426	273	490	274	264	358	297	262	321	350	331
313	320	271	462	493	0	474	265	221	277	245
232	280	443	289	211	280	288	262	170	254	501
285	493	511	508	267	239	506	320	510	303	339
291	509	371	352	308	337	229	363	287	406	287
382	276	178	299	458	356	248	314	265	446	430
430	415	506	262	415	225	396	398	443	434	432
434	369	323	251	371	185	337	170	231	483	483
404	408	420	505	229	386	195	330	550	326	378
341	190	488	470	447	393	355	202	249	348	464
509	276	137	512	257	182	190	318	220	217	196
368	218	309	346	319	324	257	308	326	381	366
321	337	289	415	415	330	365	413	501	376	496
348	215	304	402	396	396	266	583	486	688	612
725	626	702	644	247	697	374	999	398	214	211
319	297	189	222	271	213	429	323	199	346	170
241	342	374	241	371	295	284	388	478	381	278
269	212	256	329	266	315	266	246	295	134	467
101	455	170	246	273	142	231	219	368	309	175
411	15	329	257	258	250	306	229	418	459	171
318	212	278	302	302	499	276	355	359	528	367
266	363	284	310	311	239	437	171	367	284	388
139	406	360	297	453	328	157	285	242	184	477
240	483	387	308	197	202	515	298	474	190	379
291	324	237	358	224	333	450	233	481	303	410
456	431	191	362	308	304	194	319	214	362	496
358	363	280	358	343	342	241	349	378	309	263
231	321	353	310	390	347	260	308	330	298	365
333	327	402	379	342	340	449	472	305	362	322
426	356	307	365	476	219	385	257	396	385	421
231	354	372	419	422	393	348	423	387	321	

406

3463.2_1288EC31	232	250	174	269	244	237	284	251	435	270
221	282	254	249	284	322	238	330	280	265	289
356	252	373	231	253	363	275	273	366	319	337
363	333	365	374	549	213	504	306	279	215	294
213	281	429	252	195	317	295	226	269	226	429
264	471	462	473	245	265	458	324	546	263	381
284	535	380	391	272	382	232	394	299	311	265
307	385	238	410	272	445	202	353	462	409	491
488	438	469	197	469	185	468	511	459	587	427
596	454	458	211	466	234	444	228	229	580	581
303	506	519	526	253	428	221	405	300	413	483
426	261	230	506	508	416	255	266	265	383	479
311	304	263	279	258	191	233	240	277	261	188
295	177	356	401	374	383	367	422	409	446	412
405	913	426	770	765	437	817	880	701	833	668
421	259	314	825	823	834	227	374	236	377	382
328	379	348	342	258	296	363	398	999	299	283
325	299	180	222	222	284	465	262	180	268	123
221	299	402	210	392	248	353	359	352	273	234
216	213	218	267	241	308	316	267	323	258	351
184	508	192	199	262	37	239	199	357	276	233
340	90	390	235	326	233	288	310	468	452	159
268	193	295	319	251	512	231	341	403	562	468
292	266	240	301	343	214	339	211	521	303	463
189	415	519	364	518	229	229	371	272	174	468
336	565	465	280	186	216	525	391	498	213	490
365	417	181	467	231	391	529	165	534	292	732
552	517	206	480	364	299	214	323	258	461	490
338	212	327	488	486	484	283	415	456	318	272
185	343	414	354	543	458	268	354	478	373	405
424	339	592	415	396	409	372	822	310	429	431
886	509	197	676	859	163	756	260	830	828	635
377	548	404	444	369	385	316	414	361	325	

407

3600.0_1135EC04	180	239	616	149	156	111	173	139	168	147
274	91	161	158	192	126	147	243	270	262	121
136	255	26	110	278	181	179	132	176	159	57
174	156	245	139	47	712	318	102	200	155	254
214	172	0	191	30	236	161	185	199	174	167
157	256	207	215	157	147	217	189	12	142	230
204	146	298	253	160	266	203	285	378	240	253
241	295	196	264	236	345	169	216	330	221	179
201	134	161	3	145	287	277	253	304	265	141
306	272	241	874	350	209	325	341	181	340	317
0	142	86	119	206	251	85	313	233	306	317
244	140	235	100	128	91	137	174	193	217	220
226	177	299	193	164	177	913	153	441	88	296
232	167	280	278	289	288	285	299	269	268	293
360	214	205	299	268	298	293	206	257	287	226
307	958	105	285	281	276	272	186	87	169	227
121	3	142	0	967	149	310	214	299	999	140
121	206	291	141	130	173	5	65	130	38	197
115	0	199	222	216	151	0	0	106	0	135
146	144	120	100	113	296	279	89	216	162	59
60	0	176	27	113	1	204	61	32	132	0
182	80	82	161	173	161	127	114	0	201	88
145	117	161	0	46	131	200	199	0	15	317
111	111	5	425	2	176	151	149	102	234	0
129	242	31	0	230	0	148	51	224	206	261
290	0	253	191	180	221	33	13	55	60	48
0	190	65	0	164	151	87	229	61	94	213
74	287	153	73	189	321	176	298	176	94	137
56	0	37	352	115	79	117	4	187	315	298
0	299	249	120	0	283	80	7	180	67	1
114	189	312	99	274	2	274	86	0	247	248
76	208	0	129	277	123	0	218	95	2	68
277	129	351	372	205	140	167	196	133	123	

408

1220.2_1274EC17	288	312	180	960	933	378	313	298	417	313
290	339	360	433	291	325	284	267	297	365	444
427	308	380	397	297	285	354	470	345	504	361
336	335	259	325	355	191	332	455	385	371	226
301	379	385	367	245	304	360	220	376	308	337
447	318	334	311	327	340	317	256	358	239	256
263	377	308	258	280	300	315	279	266	312	408
279	286	374	275	296	326	190	236	295	332	327
331	335	361	262	333	217	350	342	363	355	330
356	337	331	163	335	187	353	288	387	348	349
249	315	316	329	467	273	268	266	266	266	287
245	284	177	338	348	290	238	288	273	335	324
308	285	255	229	339	275	156	419	267	306	223
284	432	270	290	300	274	294	327	306	336	261
302	310	323	336	323	295	312	284	341	319	335
318	144	265	313	316	314	193	199	242	178	225
309	209	210	198	141	183	290	211	283	140	999
373	323	94	344	400	313	454	291	245	346	214
302	331	315	234	284	376	340	332	455	239	300
375	223	337	370	443	318	358	384	332	217	342
253	386	283	313	372	155	285	296	362	391	202
288	0	326	174	456	381	457	329	376	363	119
284	44	380	314	355	372	235	364	326	400	334
199	356	222	333	340	313	376	222	375	396	342
186	362	370	264	314	299	349	368	206	116	432
237	391	335	269	341	234	361	253	357	125	313
0	256	182	367	364	385	345	303	370	469	368
356	363	292	333	313	257	231	281	284	362	319
372	164	313	332	321	422	297	353	412	281	312
344	278	433	331	328	324	240	270	351	296	338
291	302	331	375	361	336	361	328	220	322	288
323	308	64	270	316	165	358	165	327	353	304
230	319	308	292	283	284	215	254	217	295	

409

1269.8_1135EC44	371	408	143	392	376	363	368	265	372	277
333	424	368	427	532	522	357	349	508	476	431
376	288	356	391	311	481	423	422	447	357	397
438	429	415	517	410	127	390	422	396	362	329
316	375	444	347	165	380	366	262	283	359	575
353	395	392	387	368	394	393	284	331	277	361
273	391	376	368	285	313	325	359	398	319	371
334	403	385	385	394	449	251	396	401	370	396
404	387	411	462	415	217	417	432	418	454	355
464	421	438	106	431	197	434	292	339	475	471
262	328	329	330	400	449	255	430	274	429	437
445	266	183	427	399	433	165	267	414	558	323
279	338	373	268	373	274	108	334	353	312	257
272	275	343	311	355	345	325	359	313	401	386
339	363	305	404	394	360	388	335	379	372	387
419	109	188	335	382	375	203	291	164	287	317
300	331	282	307	170	182	269	319	325	121	373
999	505	148	281	324	368	376	213	178	508	286
304	500	579	349	366	442	305	336	389	349	290
384	185	352	392	235	513	374	355	410	178	516
265	459	242	305	376	0	335	291	423	360	214
358	0	371	318	376	301	379	344	399	421	1
179	158	428	390	337	383	240	334	374	390	401
189	322	271	320	297	335	281	121	291	359	391
200	388	431	86	314	345	283	363	113	95	437
289	360	401	175	287	207	400	209	392	90	368
22	334	59	347	306	439	362	318	369	402	443
333	419	300	396	305	238	216	288	299	399	383
328	47	315	390	339	459	200	433	431	262	264
281	262	415	387	322	361	266	338	295	343	394
346	294	340	408	381	331	365	363	141	338	346
290	337	116	360	358	72	232	39	404	355	341
322	310	252	284	233	321	120	306	253	227	

410

1273.1_1313EC43	353	326	139	321	290	313	357	294	524	315
256	337	316	399	606	639	357	344	689	327	354
333	215	314	337	318	499	311	345	479	269	461
482	473	436	529	427	177	409	352	369	318	304
250	310	450	332	170	456	282	322	235	317	414
341	329	359	365	297	388	365	319	384	355	297
312	394	237	300	298	368	269	279	464	349	394
401	341	323	345	508	424	268	355	353	434	337
361	440	357	407	361	179	476	426	466	407	442
409	451	464	220	457	169	471	207	285	405	395
275	407	410	387	346	351	121	388	239	390	391
366	204	148	401	372	338	233	196	326	314	329
295	269	336	260	325	216	193	311	272	211	245
296	214	353	344	372	355	357	388	362	407	337
400	318	351	372	376	338	377	309	363	363	377
339	209	239	348	344	348	211	356	251	317	314
271	293	288	292	243	26	304	297	299	206	323
505	999	160	5	292	357	479	220	216	377	167
330	630	381	287	456	330	411	384	341	260	190
334	223	309	347	113	577	313	264	497	199	511
211	469	305	310	358	3	255	258	384	321	194
392	142	355	291	303	239	350	303	465	377	213
279	78	413	458	371	513	239	315	429	410	444
224	408	316	336	383	328	364	149	349	384	378
55	411	445	302	324	488	253	428	239	212	469
365	384	349	195	241	289	354	186	358	159	296
2	321	189	385	263	499	417	331	434	364	419
367	430	301	395	421	292	252	244	290	407	360
345	207	366	394	386	458	154	487	457	280	247
208	249	405	418	363	339	298	359	295	384	452
352	292	344	410	384	343	350	299	291	385	330
289	340	163	385	324	221	369	190	358	362	352
324	373	336	315	289	400	291	358	303	220	



411

1275.7_1135EC06	132	195	262	133	164	216	94	208	181	134
178	101	115	90	212	171	151	207	92	147	123
171	139	166	175	164	186	139	143	176	172	92
159	172	187	123	163	280	241	208	68	149	137
147	50	9	55	180	211	126	239	159	87	93
176	134	134	111	133	31	114	232	139	242	171
222	111	197	174	258	216	68	189	169	234	194
198	165	91	142	221	202	244	157	139	167	135
176	148	105	1	172	172	171	153	173	177	136
162	150	192	293	222	269	147	230	147	173	173
177	101	106	126	312	179	117	181	245	178	182
167	142	208	130	127	99	267	139	487	128	96
235	227	200	206	125	164	306	97	185	136	232
232	203	192	206	213	196	204	229	194	255	174
142	109	103	181	188	207	192	157	164	196	171
211	281	94	118	198	199	264	111	93	128	164
204	43	174	53	310	255	338	189	180	291	94
148	160	999	52	160	94	150	237	74	29	1
107	175	95	152	254	115	0	90	148	11	170
69	184	124	200	63	173	191	157	104	203	102
43	66	46	131	15	43	139	77	108	16	139
138	497	151	113	79	154	137	160	144	96	1
276	192	101	2	208	192	223	158	141	127	224
196	171	41	206	157	119	201	156	94	178	9
192	271	101	1	138	152	159	27	325	168	197
237	125	207	179	169	163	53	122	150	216	202
146	109	481	138	144	217	85	168	100	273	212
111	48	96	130	143	349	178	237	118	145	84
108	205	81	201	60	188	153	5	169	340	291
73	245	115	243	92	222	165	161	84	209	154
32	111	107	174	189	140	300	219	2	288	101
148	169	166	161	183	155	192	287	174	179	113
258	106	355	324	334	330	306	327	381	228	

412

1281.5_1313EC36	227	194	189	371	350	311	308	189	206	296
261	148	727	263	215	224	374	197	157	376	324
335	139	256	604	192	201	610	376	251	329	221
260	236	192	225	175	148	180	376	388	319	262
242	701	268	183	122	280	323	197	319	774	269
280	254	232	243	377	304	242	303	203	230	249
274	194	211	248	275	209	785	224	165	196	238
201	190	530	225	207	239	135	332	197	238	195
181	212	221	255	209	175	208	177	208	253	214
227	211	194	240	201	156	197	818	535	209	207
213	200	200	191	332	272	172	177	191	177	178
239	205	186	259	249	252	200	822	265	316	240
192	234	316	180	257	495	248	266	243	279	96
185	474	240	214	239	258	239	265	265	259	251
200	186	199	190	184	226	211	188	195	234	209
211	142	138	196	211	187	209	190	53	210	255
125	243	225	208	166	272	212	222	222	141	344
281	5	52	999	302	308	226	193	187	247	125
727	206	269	171	139	310	33	233	231	28	194
270	599	251	298	301	217	361	441	189	2	219
336	139	241	183	358	15	263	493	253	236	100
186	0	181	230	255	280	207	360	130	257	1
133	114	268	152	277	78	154	241	179	196	229
206	202	281	231	10	633	151	476	191	169	239
755	160	254	241	188	67	498	163	29	9	211
122	144	251	135	678	201	185	189	143	2	233
0	175	133	150	485	215	183	0	191	294	250
187	228	747	249	156	196	303	169	764	237	149
156	1	750	243	185	301	671	463	373	204	207
97	169	343	169	166	222	98	207	175	230	184
233	153	172	249	199	238	212	178	3	156	243
175	231	11	183	211	140	143	91	200	216	195
214	174	168	125	86	110	193	134	145	193	

413

1282.1_1274EC17	645	372	234	413	391	935	345	164	310	191
217	479	338	336	261	299	312	209	253	376	378
374	239	317	559	248	328	347	361	339	387	318
333	352	271	299	304	174	283	544	331	323	237
264	297	312	346	224	313	327	243	321	334	284
348	305	308	301	323	616	291	224	257	223	295
242	274	320	303	204	257	309	309	254	219	314
226	239	302	229	262	267	214	289	272	267	274
280	268	290	308	274	223	305	306	295	272	267
276	274	268	167	278	135	279	334	312	288	291
203	233	234	243	345	248	266	279	285	275	213
249	224	227	261	242	229	230	315	334	341	221
253	361	256	257	334	324	164	303	276	294	164
261	405	231	222	219	248	227	274	278	289	241
227	258	210	261	261	249	263	227	261	264	277
236	129	316	217	284	285	253	213	30	212	237
121	33	207	207	119	237	244	271	222	130	400
324	292	160	302	999	345	330	175	188	469	65
267	248	299	193	207	304	167	324	388	228	417
478	203	482	490	338	259	320	395	254	4	295
297	294	181	234	365	0	272	255	254	375	207
232	0	214	198	344	251	326	264	269	346	44
221	82	607	262	244	293	148	270	271	273	329
167	218	182	310	205	314	246	91	212	290	261
220	285	323	168	199	264	275	255	142	57	305
182	219	284	322	298	10	265	251	280	28	250
0	245	137	268	279	259	234	131	250	321	318
220	261	294	272	228	258	246	338	321	278	191
182	17	189	280	259	320	294	316	340	270	253
276	322	303	242	254	235	184	190	171	230	289
188	192	237	264	249	260	337	250	36	252	227
194	231	2	256	244	90	259	8	271	273	213
231	199	242	230	168	244	168	219	191	187	

414

1291.0_1185EK01	348	449	192	340	322	343	999	191	391	790
292	320	404	537	313	361	845	262	310	389	389
411	212	329	399	302	436	393	421	403	474	404
399	391	253	321	352	220	347	455	379	345	316
269	375	346	331	187	299	370	252	255	348	317
385	305	327	315	278	346	316	267	354	285	275
318	325	279	272	306	262	359	256	290	255	344
317	319	389	304	299	327	205	335	330	315	253
259	326	290	292	278	203	355	305	340	326	314
320	331	299	185	289	216	318	299	356	307	307
208	325	325	333	375	340	318	270	260	275	267
277	225	159	318	322	284	250	308	231	357	289
284	305	312	164	325	366	170	394	295	277	202
253	385	279	238	259	287	253	274	260	328	284
278	266	255	319	299	241	296	255	324	317	344
283	163	219	306	300	297	241	202	48	229	229
239	113	178	180	182	201	240	213	284	173	313
368	357	94	308	345	999	426	209	806	339	223
366	321	388	236	280	327	270	304	416	280	458
358	307	383	433	415	301	443	466	322	143	364
308	358	217	221	398	142	217	377	343	389	176
239	0	265	235	420	303	389	296	328	338	30
252	87	364	341	314	303	269	330	323	381	347
332	297	249	284	222	391	322	191	305	343	296
194	346	322	248	243	303	366	305	259	176	376
218	291	334	225	374	240	307	218	301	134	294
2	316	206	330	342	297	330	160	342	378	358
284	320	355	313	267	279	344	253	350	305	305
295	189	337	364	318	370	270	350	417	277	300
184	250	359	255	261	265	207	266	287	242	473
313	276	263	340	356	299	343	263	151	307	278
268	283	134	306	282	145	261	159	302	291	273
237	277	249	270	253	280	211	263	240	200	

415

1293.1_1313EC75	390	357	8	429	398	354	426	305	974	313
368	434	387	422	525	522	381	367	458	408	543
538	240	584	372	306	471	365	401	725	524	678
725	699	482	556	738	6	651	399	481	350	403
389	357	648	402	198	428	440	272	394	344	482
428	594	570	582	352	371	567	357	667	311	537
350	718	581	548	309	414	324	581	463	453	349
385	508	318	426	437	462	215	411	476	624	646
643	659	639	278	642	131	671	658	675	657	642
655	673	699	117	714	189	708	255	342	641	641
392	621	626	633	443	391	274	661	324	658	522
428	259	322	602	570	407	315	272	419	359	467
358	321	305	372	326	193	119	394	307	307	151
365	183	398	449	422	403	420	457	412	478	371
431	516	386	588	606	450	570	495	650	566	670
432	94	297	561	535	559	264	423	178	405	437
350	336	404	438	101	247	299	429	465	5	454
376	479	150	226	330	426	999	238	226	501	21
338	459	551	205	383	362	480	468	517	345	278
328	142	316	439	389	479	291	379	467	300	523
338	745	80	258	424	148	356	270	589	416	270
430	0	444	284	359	315	458	266	669	624	33
240	165	420	452	281	671	82	374	593	715	560
392	424	288	234	463	255	452	164	482	319	557
161	608	617	329	519	383	261	436	168	0	634
390	585	571	357	257	268	638	388	601	54	534
257	514	146	589	297	541	642	320	681	431	584
584	635	282	558	363	289	125	306	346	551	505
327	95	317	581	617	712	424	474	642	309	286
238	285	609	533	569	531	266	368	474	441	656
412	394	486	621	589	482	538	555	205	389	423
423	429	88	541	536	126	528	7	542	559	562
330	401	281	257	226	322	218	328	251	301	

416

1296.5_1191EC10	136	192	107	246	263	131	209	955	246	321
300	185	262	211	251	283	226	260	170	263	155
191	175	222	130	171	245	239	220	228	279	260
232	238	202	284	243	93	197	210	225	234	306
261	203	226	168	187	298	242	218	240	164	256
224	229	220	212	221	156	213	655	217	580	219
624	215	219	218	575	602	194	229	316	640	216
576	294	202	234	235	323	166	330	243	297	264
277	254	248	92	269	190	233	244	229	240	244
242	247	237	146	257	287	237	235	149	238	241
225	216	219	242	289	229	108	288	240	288	198
234	226	273	207	202	225	250	287	256	255	252
242	170	242	258	172	165	87	180	246	281	116
232	70	516	535	547	515	535	574	506	433	513
530	221	166	203	232	233	211	229	243	250	257
243	60	65	201	222	200	305	271	232	267	273
256	144	271	269	93	145	227	323	262	65	291
213	220	237	193	175	209	238	999	209	221	0
281	138	197	133	212	234	37	180	206	228	153
98	122	161	268	305	326	212	230	188	0	255
253	234	169	191	243	170	266	162	187	181	63
239	154	195	264	160	144	246	196	113	209	0
209	426	148	112	157	237	135	249	145	233	496
198	85	207	135	256	141	676	0	122	171	195
54	264	222	238	245	579	155	223	205	96	285
213	286	222	159	144	175	271	255	233	101	196
238	243	192	240	131	245	173	180	220	270	231
289	231	216	223	476	190	87	197	230	243	263
394	386	62	233	257	244	153	147	286	183	162
145	192	227	232	256	574	379	529	214	562	266
445	491	235	247	269	522	302	273	12	92	499
203	531	429	210	246	91	255	196	211	253	232
439	353	334	306	268	252	260	277	270	214	

1316.0_1313EC36	203	242	218	270	321	198	806	137	244	970
266	10	252	306	190	192	858	169	223	312	293
325	154	189	297	237	327	204	263	187	344	205
199	177	163	228	141	202	171	318	286	242	272
273	242	177	257	49	282	328	123	195	193	198
277	201	206	207	275	223	211	203	176	194	197
267	162	143	192	245	168	215	143	166	154	290
98	193	222	135	162	198	120	265	225	244	232
236	190	204	243	245	210	273	144	271	175	193
146	278	269	172	258	209	252	210	291	125	125
126	167	166	170	321	232	223	167	124	200	155
183	193	117	212	144	86	79	241	186	220	113
151	178	282	104	223	222	166	288	241	267	169
123	283	207	177	209	208	199	218	195	197	190
192	173	176	184	149	199	191	173	195	198	199
238	135	78	145	224	184	193	180	147	227	202
224	16	189	185	140	178	149	199	180	130	245
178	216	74	187	188	806	226	209	999	140	198
200	137	265	174	138	279	79	216	247	171	316
251	184	277	288	246	199	289	372	252	149	93
234	91	76	110	241	145	246	311	127	274	85
98	0	140	121	287	246	239	232	140	216	56
114	2	226	173	279	94	180	202	161	178	236
208	183	198	187	79	231	23	161	241	265	82
124	220	251	168	84	24	270	164	206	123	240
174	134	327	143	244	190	201	101	194	52	135
0	258	0	230	272	207	206	200	211	264	221
141	84	236	184	74	178	206	181	144	143	75
161	217	226	253	196	206	186	184	311	187	195
149	185	294	219	107	215	82	154	186	146	387
163	141	125	240	275	201	196	105	38	192	148
59	116	57	194	149	0	164	23	197	155	79
183	37	196	181	145	148	144	153	127	106	

418

1317.6_1313EC75	420	471	38	378	353	508	339	238	489	190
272	940	357	420	411	401	328	274	350	372	400
606	303	575	390	275	386	407	477	482	431	494
482	492	316	355	383	44	340	384	407	369	279
277	390	496	341	315	288	325	286	449	321	463
407	312	323	313	355	385	304	244	321	256	493
255	374	502	507	246	253	325	487	319	294	307
307	327	369	289	336	320	224	264	296	314	313
324	334	334	327	356	233	360	400	367	366	317
362	347	342	59	330	196	333	312	359	390	383
245	291	292	300	408	307	346	391	344	387	306
282	283	289	351	327	326	254	314	290	373	268
317	356	304	328	429	268	59	343	343	355	247
278	304	253	245	269	250	235	259	257	319	262
258	297	235	348	331	261	319	258	321	304	342
297	36	383	293	321	305	215	303	132	299	296
301	227	258	308	39	271	253	346	268	38	346
508	377	29	247	469	339	501	221	140	999	10
259	376	473	235	316	319	205	504	620	331	496
318	97	482	568	330	372	323	431	308	257	380
287	380	193	240	395	114	238	290	452	375	322
357	0	293	229	378	290	409	328	377	356	4
184	98	398	450	271	353	133	321	463	374	357
106	249	227	337	337	346	306	1	311	299	334
202	363	412	97	266	301	276	306	151	6	416
274	287	333	395	327	191	332	265	344	39	383
6	271	109	283	326	281	328	191	352	397	376
296	384	311	356	286	329	245	386	396	384	251
399	38	273	328	311	443	237	346	423	370	328
281	380	349	322	311	292	273	233	228	207	424
249	243	283	338	322	266	457	314	123	329	270
262	274	139	359	295	164	342	11	342	334	300
221	265	251	264	228	316	150	275	243	275	



419

1318.4_1313EC75	168	157	263	239	203	64	223	2	24	249
944	5	108	362	160	203	197	227	205	100	142
152	193	136	221	193	141	172	96	169	145	23
181	89	114	172	100	320	212	197	199	157	275
244	236	29	115	3	141	162	147	146	103	138
111	144	152	150	111	183	154	187	100	272	149
193	137	137	143	256	149	173	130	141	103	202
123	91	635	117	93	173	102	229	153	184	173
158	151	149	44	156	273	129	150	130	141	156
139	131	126	235	120	245	127	147	158	165	167
164	105	102	94	103	155	86	209	137	206	219
144	116	202	138	123	143	99	194	128	182	120
109	154	264	172	27	235	247	19	204	164	222
135	234	157	172	159	178	155	179	163	169	144
121	134	168	149	139	170	149	116	137	158	155
197	240	105	125	150	141	201	158	1	153	153
9	11	167	177	211	92	195	170	123	197	214
286	167	1	125	65	223	21	0	198	10	999
50	48	135	196	221	18	13	306	55	231	158
214	145	38	209	70	43	236	446	187	191	179
3	132	4	106	196	0	106	169	215	91	2
231	0	211	610	593	153	10	285	20	164	79
103	248	197	25	272	218	21	202	247	65	171
222	128	280	226	304	267	7	99	215	187	35
4	214	193	11	149	82	607	68	112	344	200
12	17	159	105	168	4	85	333	88	190	191
0	136	0	16	144	193	124	2	21	45	195
15	261	261	157	84	194	261	170	177	65	174
143	6	82	203	66	227	16	174	102	179	235
35	172	291	162	11	84	73	70	182	143	264
10	13	136	251	256	171	181	152	13	206	188
190	212	321	22	129	1	13	0	153	18	143
147	62	159	203	128	159	117	142	174	118	

420

1326.5_1274EC17	325	294	128	336	357	283	366	273	300	261
309	198	929	340	319	347	329	295	362	382	362
339	132	254	531	266	267	781	382	325	323	281
342	333	307	346	288	132	254	387	376	368	263
308	635	343	325	99	351	352	232	301	732	294
346	311	300	312	337	290	322	336	283	295	276
308	277	255	276	314	278	728	269	332	258	271
281	296	527	223	259	279	159	333	286	294	303
299	294	294	321	309	209	297	294	301	256	293
267	306	325	168	310	150	324	702	540	267	265
221	283	283	280	333	296	151	342	238	321	258
284	183	114	270	289	295	214	699	298	314	263
243	256	233	184	245	434	164	298	256	191	144
243	444	274	270	299	326	293	316	316	303	286
280	270	279	272	264	270	286	221	261	313	262
273	114	6	209	288	283	183	282	119	250	290
296	250	273	285	110	150	217	241	221	115	302
304	330	107	727	267	366	338	281	200	259	50
999	325	335	226	368	369	255	313	272	200	167
347	486	298	325	220	362	378	337	293	229	343
287	302	202	170	385	172	315	460	327	358	167
313	0	284	277	263	336	309	377	282	324	0
95	172	266	296	362	225	249	316	342	291	320
166	326	406	215	282	575	301	356	364	263	280
658	260	310	306	220	278	406	311	117	4	282
246	310	317	147	611	358	314	203	242	1	246
1	304	101	344	512	308	270	352	288	314	294
260	311	668	283	306	165	327	122	670	303	270
166	295	759	254	284	389	552	546	397	162	125
114	105	378	286	248	313	215	287	271	270	293
306	291	240	322	248	320	268	214	98	303	254
238	283	60	307	218	231	237	134	280	310	239
233	217	177	142	101	181	168	167	161	145	

421

1338.0_1313EC75	339	264	3	267	334	237	321	233	454	207
348	273	363	420	632	950	259	340	708	386	365
347	179	390	268	275	552	334	289	472	294	442
425	447	539	493	432	0	379	282	389	272	382
300	334	428	309	201	466	443	101	241	326	407
239	343	349	353	392	328	354	214	418	238	341
218	490	346	349	187	406	303	345	455	424	309
295	352	253	376	436	452	69	415	423	397	371
424	451	423	380	432	138	447	405	466	411	437
411	435	436	0	436	138	448	174	251	430	426
258	387	386	372	218	354	172	435	201	439	375
369	199	252	362	379	368	111	204	345	323	397
181	219	249	292	280	187	2	322	225	252	171
167	186	340	405	344	332	347	353	330	333	355
393	413	358	397	386	369	402	345	342	381	395
373	0	201	358	388	378	167	375	185	350	362
325	363	299	349	142	341	258	342	299	0	331
500	630	175	206	248	321	459	138	137	376	48
325	999	378	313	425	384	297	384	296	261	176
372	136	283	320	107	690	281	272	610	309	493
257	481	197	307	343	2	300	216	385	340	159
393	0	434	349	277	302	272	352	411	408	0
115	148	314	443	250	423	211	326	424	468	475
209	479	301	226	262	230	429	146	397	280	403
127	384	480	332	315	348	102	482	143	114	412
339	387	321	192	189	317	413	201	383	190	317
0	381	0	395	207	518	441	273	452	301	388
396	456	231	349	355	182	136	187	217	355	458
263	219	397	323	392	437	162	468	430	215	201
179	183	447	410	317	473	191	349	347	370	452
398	369	345	410	374	368	378	324	183	383	404
359	368	197	372	329	231	386	192	385	405	369
307	380	207	261	183	277	175	248	174	239	

422

1352.5_1274EC17	354	399	217	354	378	330	388	275	547	256
276	398	398	398	424	456	357	289	395	438	350
372	238	385	280	237	429	390	311	543	348	556
531	508	447	504	561	214	574	314	382	289	313
291	276	714	340	219	377	356	282	330	257	731
324	500	502	503	334	310	513	264	488	238	391
242	526	396	394	241	304	281	399	361	317	322
325	439	319	347	427	416	259	375	395	464	510
520	483	503	339	505	141	476	462	472	534	464
541	468	489	258	530	141	522	258	285	564	568
305	483	483	471	324	450	251	474	281	474	633
518	241	229	643	593	549	227	279	368	409	352
296	327	263	271	283	191	208	309	288	255	175
278	195	324	332	346	318	330	384	359	396	355
339	394	304	426	432	346	410	405	484	444	494
343	205	187	413	401	419	190	334	159	327	353
347	302	327	333	243	256	297	374	402	199	315
579	381	95	269	299	388	551	197	265	473	135
335	378	999	259	303	386	265	328	346	435	227
341	86	335	415	275	438	255	287	403	249	491
207	535	110	261	309	2	300	254	654	296	199
377	5	352	239	287	230	302	318	525	539	76
240	102	326	483	234	493	104	265	464	534	408
302	339	287	280	291	267	323	116	317	282	698
142	404	477	267	375	292	241	334	136	74	438
274	427	486	201	262	320	507	282	469	54	442
17	428	142	482	243	424	511	235	507	294	448
436	622	232	443	314	242	200	238	282	453	404
209	225	349	500	490	493	215	384	472	261	225
150	248	480	475	405	392	257	301	306	338	468
330	297	366	450	459	365	391	355	143	464	327
338	317	5	391	425	156	340	175	372	379	416
262	335	209	255	164	238	152	252	142	259	

423

1364.2_1313EC11	248	214	215	223	224	216	236	190	232	204
331	213	250	257	384	355	211	293	346	321	199
221	245	224	173	482	339	300	230	276	225	266
278	272	300	299	249	252	277	208	261	221	283
272	244	247	188	82	370	254	154	263	243	257
234	252	252	228	258	173	245	312	159	277	240
287	230	244	242	244	277	257	243	278	330	244
264	301	253	265	257	347	177	255	414	319	218
243	256	227	296	237	253	231	246	245	246	253
269	234	228	278	264	147	254	256	255	271	237
218	253	237	235	256	253	77	340	192	352	249
248	216	245	205	172	233	49	238	249	253	203
204	194	298	235	254	166	279	248	307	248	282
173	190	270	293	272	284	261	297	263	297	306
267	242	288	245	250	283	246	233	246	236	276
297	246	17	251	247	234	216	363	245	323	388
316	196	334	321	205	200	209	241	210	222	234
349	287	152	171	193	236	205	133	174	235	196
226	313	259	999	193	199	239	211	164	61	100
237	173	239	279	127	365	257	232	282	223	288
209	229	107	182	229	0	255	215	264	183	98
242	0	238	286	216	205	260	307	257	277	16
24	92	178	226	188	219	8	204	282	214	325
154	315	301	254	159	191	268	5	205	212	198
89	307	247	221	204	156	202	261	239	199	243
324	252	194	162	167	490	215	154	223	4	177
0	231	0	209	175	251	244	272	212	291	240
216	232	252	203	246	129	223	131	208	234	205
143	150	267	266	202	229	145	245	255	127	118
160	175	288	252	242	239	185	183	189	208	239
181	234	259	253	223	229	204	198	114	278	239
138	259	0	228	229	3	212	0	219	218	170
241	161	112	112	44	119	186	224	127	126	

424

1372.9_1313EC75	267	288	150	299	302	219	280	262	353	278
328	313	294	358	716	469	301	887	489	302	288
272	224	299	243	318	401	261	248	358	270	359
351	356	496	582	359	238	345	279	306	255	340
326	326	461	271	144	451	434	223	276	270	416
281	359	322	328	309	280	327	339	333	291	346
328	371	387	347	282	413	251	378	465	255	443
327	352	310	542	363	468	215	473	439	391	342
342	352	354	243	364	159	393	394	399	503	356
505	385	385	212	402	202	391	199	253	493	511
278	321	327	319	272	400	184	447	221	450	421
427	273	220	439	402	406	157	247	288	354	385
222	206	311	284	328	178	217	330	294	181	328
231	157	330	358	333	354	328	355	337	380	379
421	431	412	419	422	470	416	388	415	407	433
490	223	45	389	405	396	211	377	192	390	418
305	280	405	345	199	238	311	371	392	216	284
366	456	254	139	207	280	383	212	138	316	221
368	425	303	193	999	293	312	435	290	379	167
318	92	307	281	170	467	301	289	513	252	573
166	458	37	186	320	1	320	248	440	331	189
462	0	430	298	294	367	325	255	274	369	71
146	154	268	373	375	372	138	339	406	352	412
272	321	319	296	326	264	336	84	391	442	331
40	378	424	248	282	396	195	378	81	146	376
273	348	394	204	214	198	325	207	305	143	330
0	354	0	360	225	514	345	287	339	322	444
290	450	213	331	386	268	207	260	257	325	431
138	69	189	408	321	384	148	361	378	256	152
176	267	373	364	286	384	204	297	344	338	360
347	381	465	377	378	287	324	397	312	359	379
326	366	5	291	411	3	218	5	404	326	378
337	357	271	234	182	291	108	241	154	174	

425

1378.1_1313EC75	317	289	208	326	348	310	327	256	366	278
309	275	424	388	339	370	334	268	362	940	500
342	186	346	391	335	318	399	336	360	347	352
374	384	339	419	344	206	335	324	473	337	366
305	363	353	322	140	345	338	186	409	315	346
280	333	339	350	359	451	331	286	332	279	331
292	357	306	336	250	300	301	316	350	304	356
358	374	334	324	278	330	170	290	364	386	345
349	397	366	655	368	165	349	330	357	343	383
351	344	345	170	334	120	344	269	335	353	345
247	329	331	333	333	361	221	343	244	341	328
315	271	206	326	328	327	204	288	307	403	350
256	283	289	218	316	327	171	342	269	313	165
208	286	326	355	298	293	297	320	332	332	323
347	305	285	320	296	281	337	299	280	312	300
278	175	148	277	329	310	211	307	224	295	312
308	212	321	315	176	254	231	295	248	151	376
442	330	115	310	304	327	362	234	279	319	18
369	384	386	199	293	999	195	325	339	249	258
418	185	276	355	283	388	316	320	338	195	407
404	356	268	583	457	0	310	279	327	340	152
345	0	283	261	293	261	280	389	345	369	37
100	166	451	265	285	295	222	334	291	354	362
235	288	265	251	294	305	365	226	296	333	351
176	301	345	268	307	372	272	353	202	88	323
261	366	336	164	279	255	371	304	344	68	258
329	311	157	328	297	391	340	277	351	330	350
351	362	293	350	325	171	218	185	334	372	355
201	21	269	349	375	315	284	345	366	190	192
259	187	329	313	256	373	164	349	288	278	327
307	329	288	343	311	342	301	304	101	289	317
307	264	78	308	299	181	281	134	321	340	339
293	286	223	238	197	239	219	236	209	184	

426

1381.0_1313EC75	312	245	0	319	232	163	270	170	504	230
199	296	249	296	376	400	202	263	432	340	817
362	113	336	212	268	355	299	419	361	436	316
340	317	351	318	431	0	409	240	388	277	192
199	252	315	414	207	373	410	204	231	253	356
466	291	317	291	205	385	287	166	390	171	293
179	399	267	288	188	232	206	273	304	233	302
215	734	172	311	274	367	171	193	402	310	305
297	294	319	275	302	95	342	558	354	401	300
403	317	326	0	324	110	320	202	313	419	420
228	354	356	376	452	299	212	275	239	275	286
246	197	193	311	334	277	143	146	280	260	369
222	178	209	238	204	89	0	370	282	278	144
220	110	255	270	253	244	251	268	231	296	240
330	323	140	468	491	224	428	338	452	456	446
215	0	130	449	443	437	190	272	158	272	295
226	356	274	292	0	11	247	284	353	0	340
305	411	0	33	167	270	480	37	79	205	13
255	297	265	239	312	195	999	258	357	58	24
275	12	246	304	312	379	117	155	370	325	267
0	398	4	237	355	0	244	204	325	420	295
236	0	249	210	321	357	469	203	516	339	0
0	11	421	252	212	321	5	274	323	411	340
209	408	249	201	276	145	249	6	379	297	266
109	300	269	182	576	305	212	330	136	0	428
262	535	272	112	131	216	310	426	312	0	233
256	289	258	353	229	417	368	228	382	538	389
550	365	158	557	377	149	150	165	180	561	348
161	20	227	320	327	393	184	282	330	209	168
202	162	331	326	595	314	183	227	254	158	308
457	330	331	319	317	302	279	353	140	251	305
333	371	18	481	357	88	486	4	443	437	599
207	320	207	111	1	138	8	178	60	137	



427

1394.9_1274EC17	384	243	1	351	370	336	304	315	472	217
371	418	332	370	491	438	299	439	375	371	320
404	305	539	357	292	480	361	302	458	315	423
452	438	485	570	448	0	392	375	442	278	349
315	364	443	302	139	388	360	317	379	341	428
290	390	417	408	372	397	404	297	395	337	603
313	407	590	610	310	335	313	587	419	339	313
370	293	315	435	375	468	211	368	376	413	428
378	403	406	224	420	127	406	423	409	424	388
424	401	413	0	411	235	414	287	322	466	458
316	356	359	370	339	395	241	509	292	508	382
381	277	287	449	427	397	236	304	409	385	401
286	307	303	298	239	242	0	294	250	277	270
284	253	304	361	321	324	339	373	335	412	375
351	367	340	417	414	432	412	359	392	385	403
390	0	377	359	390	381	259	362	139	397	359
321	246	358	364	0	234	329	388	359	0	332
336	384	90	233	324	304	468	180	216	504	306
313	384	328	211	435	325	258	999	426	366	292
482	171	420	443	245	415	302	357	474	305	576
311	483	131	228	420	3	269	294	410	308	205
509	0	446	311	315	273	313	248	400	444	0
180	154	395	450	316	476	90	345	537	398	401
309	324	267	267	313	289	343	163	403	342	372
170	474	475	250	293	333	250	396	137	1	476
358	318	374	397	272	288	379	304	360	2	373
2	369	130	334	274	421	387	215	389	306	424
343	444	304	358	277	342	145	400	316	353	419
296	63	287	349	364	493	225	391	431	342	324
251	387	460	397	294	343	218	305	401	302	488
288	287	387	418	414	351	403	404	130	361	378
327	350	12	330	383	123	321	136	397	329	348
354	310	324	239	274	312	260	306	259	260	

428

1403.1_1274EC17	372	344	166	473	405	403	416	242	519	343
300	577	370	427	358	388	408	307	323	414	488
948	260	653	411	299	417	408	569	415	639	419
439	414	371	438	443	144	416	431	479	489	349
312	401	478	509	196	399	436	307	392	399	452
538	407	396	399	536	360	391	326	441	294	504
304	475	506	508	326	376	357	509	304	363	381
320	287	381	346	399	413	283	351	350	468	450
453	453	455	313	457	206	416	381	436	463	460
469	423	416	120	449	221	414	322	399	474	472
375	378	372	417	612	372	311	394	360	393	375
376	335	410	458	422	353	305	290	360	427	348
364	375	295	423	490	323	124	570	402	438	214
320	336	363	387	382	366	363	412	374	426	369
337	383	326	414	416	361	408	373	440	410	435
341	116	314	363	411	402	259	377	124	421	393
388	259	396	368	105	359	334	478	352	106	455
389	341	148	231	388	416	517	206	247	620	55
272	296	346	164	290	339	357	426	999	294	350
337	264	392	437	538	307	399	477	316	216	412
378	389	169	243	427	215	251	306	467	517	192
272	0	331	205	413	387	558	327	391	455	41
231	131	427	362	373	437	224	444	409	465	415
256	242	252	301	253	356	312	128	449	366	351
244	379	530	207	331	360	330	305	244	134	535
303	308	437	327	324	263	447	296	398	110	421
203	310	246	348	392	396	397	258	420	600	473
337	463	332	375	307	324	288	349	399	384	371
431	46	294	407	383	428	287	347	463	351	337
436	336	429	383	400	407	256	341	363	321	375
302	271	397	416	406	386	470	426	188	305	366
354	375	84	343	396	107	317	169	407	393	379
297	298	284	306	325	345	216	325	289	268	

429

1410.5_1313EC75	205	257	106	275	244	239	280	242	330	261
295	236	230	390	339	319	254	287	183	209	268
289	199	271	195	218	352	295	204	237	207	226
242	245	359	358	281	0	258	276	314	190	293
191	259	549	219	77	283	223	200	218	227	581
189	257	236	240	234	278	232	302	275	237	329
223	265	256	338	246	228	258	284	285	203	216
230	281	294	313	283	337	139	331	346	261	247
259	249	239	232	247	161	257	317	261	370	246
375	264	263	0	263	166	269	306	253	377	376
292	305	288	274	265	343	209	315	179	327	412
425	248	191	482	442	475	147	288	220	260	289
161	299	259	238	206	113	85	164	281	231	112
232	159	217	188	290	225	236	329	281	283	292
262	281	283	273	286	271	282	307	296	294	318
295	0	217	299	298	297	220	320	9	328	326
314	261	322	309	0	194	210	381	273	0	239
349	260	11	28	228	280	345	228	171	331	231
200	261	435	61	379	249	58	366	294	999	121
209	2	256	249	185	287	287	262	314	4	370
219	337	69	43	271	1	195	307	490	237	142
342	0	304	271	240	166	199	300	227	278	0
2	55	245	273	276	207	188	251	139	272	254
154	114	220	235	192	241	232	0	255	206	529
5	221	335	135	279	191	222	350	120	2	351
172	320	281	236	220	207	240	267	168	0	197
15	245	1	237	227	347	326	152	299	219	311
340	476	242	266	196	145	28	232	355	322	319
288	42	286	224	217	223	176	235	217	188	89
179	223	213	263	281	240	217	235	306	278	201
246	262	301	175	211	288	274	309	253	155	304
258	234	79	260	296	0	236	6	283	281	286
198	281	284	197	293	234	199	254	237	106	

430

1414.0_1274EC17	495	368	162	320	342	443	458	188	289	333
321	417	305	333	230	276	438	237	168	393	267
374	306	331	408	265	351	344	304	351	357	321
357	321	264	255	277	168	287	480	348	287	354
288	323	294	227	323	285	342	284	409	351	279
274	288	277	277	329	379	284	288	251	292	353
326	293	335	356	257	293	315	341	261	248	391
291	274	316	259	228	299	215	379	281	303	286
283	307	293	220	293	257	281	269	285	266	294
290	283	270	176	294	178	299	326	357	282	271
163	213	215	221	252	245	470	296	229	286	169
227	291	282	255	230	208	176	315	315	336	222
231	343	338	265	316	355	176	189	324	283	261
237	444	274	287	304	293	290	316	289	306	314
251	243	241	258	248	277	263	231	266	262	280
311	133	280	234	277	259	266	233	137	259	277
139	4	245	244	123	198	253	278	234	135	300
290	190	170	194	417	458	278	153	316	496	158
167	176	227	100	167	258	24	292	350	121	999
281	191	447	457	321	270	318	426	106	7	260
361	229	144	182	283	59	268	389	265	222	315
154	0	230	177	307	275	210	280	199	304	93
338	158	396	145	242	276	355	249	216	233	323
179	115	148	330	204	312	179	160	156	352	193
251	310	285	2	170	164	278	173	182	191	340
195	70	300	285	319	4	268	250	283	119	321
0	195	126	169	325	104	203	104	222	239	298
203	229	336	282	147	345	247	345	313	261	120
203	1	123	301	223	327	238	182	375	320	389
171	321	333	280	197	301	240	222	149	258	347
88	208	241	307	321	293	338	212	8	211	249
124	280	106	252	243	39	197	126	262	241	184
265	167	285	307	286	295	145	265	262	239	

431

1419.8_1313EC75	582	264	158	392	351	483	358	205	313	374
297	259	378	364	323	352	348	294	354	467	434
354	185	379	447	277	417	405	336	351	309	337
374	379	303	390	301	151	293	436	373	370	258
264	323	347	321	143	316	316	203	407	334	323
324	311	317	310	310	487	316	246	254	294	416
254	277	432	393	296	248	299	387	297	269	336
316	290	299	291	379	317	167	319	317	253	230
238	280	265	342	279	126	389	295	384	293	268
307	398	374	94	356	150	387	257	299	309	306
275	247	247	248	301	423	232	327	228	323	303
384	269	164	290	277	271	175	246	407	378	290
270	331	298	229	340	286	90	386	299	333	147
206	398	313	251	305	317	295	299	326	312	292
297	243	296	331	314	247	317	248	226	290	255
261	146	203	227	337	318	177	248	221	242	249
241	254	245	239	116	127	234	269	216	146	375
384	334	69	270	478	358	328	98	251	318	214
347	372	341	237	318	418	275	482	337	209	281
999	17	641	621	191	338	351	350	346	227	390
248	344	210	231	379	0	294	247	319	362	170
346	0	277	271	254	226	311	360	316	351	87
96	1	499	335	280	291	65	273	399	294	354
153	334	251	254	257	270	285	72	286	304	256
281	311	347	140	247	306	219	329	123	2	313
306	315	318	157	265	236	296	198	232	2	237
213	326	136	382	266	369	259	185	290	286	304
266	307	274	274	244	158	149	147	271	302	309
204	27	227	273	284	333	155	332	341	183	197
197	144	336	286	242	273	258	316	296	272	396
243	259	248	287	283	254	267	263	106	298	250
265	259	1	351	254	43	271	2	342	333	260
226	279	187	159	100	180	104	196	139	159	

432

1436.0_1313EC36	237	300	106	254	274	239	307	124	136	210
237	135	503	263	171	181	254	197	85	293	278
256	135	149	404	219	116	440	319	227	280	96
260	202	178	179	167	126	127	325	281	219	271
280	485	14	159	197	307	296	243	311	594	127
226	256	255	268	309	219	267	264	133	236	244
249	145	189	247	259	212	557	217	190	136	330
177	173	501	165	183	265	214	254	207	237	221
181	191	240	62	198	175	202	140	203	202	194
228	205	198	179	190	160	205	570	572	193	217
160	148	148	142	243	250	228	231	193	230	94
235	210	186	187	151	85	149	562	247	308	188
202	221	241	193	258	474	178	86	274	187	145
226	521	222	265	254	257	265	277	259	238	232
184	146	155	165	160	180	172	150	214	223	213
209	148	6	151	178	166	165	203	235	202	258
4	0	249	118	144	136	182	212	213	144	223
185	223	184	599	203	307	142	122	184	97	145
486	136	86	173	92	185	12	171	264	2	191
17	999	249	195	289	137	407	315	30	142	84
222	76	35	142	222	23	274	346	108	168	175
105	0	80	188	282	258	167	268	118	249	147
117	225	236	15	282	8	248	241	20	112	273
184	4	242	190	107	598	2	411	137	298	6
574	146	133	1	117	154	468	1	216	142	194
155	0	251	127	570	121	211	99	196	6	209
0	212	110	1	538	165	100	279	110	164	234
100	8	595	138	116	167	375	182	560	18	124
64	0	523	248	172	218	552	397	312	148	184
104	150	316	199	135	232	139	169	174	135	99
3	123	199	236	251	189	112	132	0	126	215
2	258	5	227	185	163	4	65	187	70	154
185	37	164	108	79	132	0	141	141	99	

433

1440.3_1274EC17	448	350	144	393	349	486	383	236	302	234
240	464	364	358	299	310	335	270	280	346	334
414	257	346	393	294	340	426	355	404	354	356
404	396	258	309	262	148	272	414	372	382	269
259	345	353	288	265	343	314	252	402	328	300
339	302	330	312	385	422	307	253	239	274	506
248	254	517	489	291	249	317	480	272	219	295
271	275	372	308	284	304	202	277	298	266	241
261	240	237	274	245	225	423	297	415	258	232
259	412	424	117	412	176	422	321	332	275	286
241	223	223	227	333	418	376	281	250	285	287
360	354	209	249	248	258	187	336	330	348	234
245	389	295	250	419	387	115	402	364	401	184
256	473	346	265	348	347	317	319	315	299	286
254	242	233	337	318	256	325	221	250	313	247
289	120	264	236	354	333	227	227	120	263	246
275	209	231	222	88	163	266	256	218	120	337
352	309	124	251	482	383	316	161	277	482	38
298	283	335	239	307	276	246	420	392	256	447
641	249	999	791	295	332	349	400	273	239	359
304	324	151	214	387	190	257	250	328	334	255
222	0	227	198	354	253	333	340	282	354	54
209	81	431	359	266	266	137	304	394	252	326
232	247	209	313	235	332	291	80	233	293	244
257	320	285	155	215	284	290	283	205	135	307
217	239	348	267	340	186	236	228	238	85	228
0	355	66	352	326	244	220	185	243	315	328
215	268	301	258	235	259	308	292	333	291	218
272	16	261	271	237	325	244	304	352	271	253
299	284	315	255	221	247	226	317	162	264	353
221	227	241	297	271	267	363	254	124	291	247
235	288	72	345	248	28	281	2	351	301	219
234	252	264	243	199	274	207	252	228	183	

434

1450.0_1313EC75	487	387	134	423	406	527	433	297	428	300
324	524	438	397	333	357	386	263	325	424	417
477	288	464	415	305	412	469	394	502	416	485
521	527	351	365	373	166	384	441	454	443	316
308	372	425	286	285	372	372	306	481	377	370
394	395	404	399	368	418	392	311	357	352	582
310	382	574	567	350	308	375	549	356	309	374
308	326	401	318	347	351	205	369	337	334	342
356	350	348	330	372	164	483	401	474	326	331
329	489	476	92	457	203	473	369	380	359	351
323	319	322	331	388	418	364	386	260	384	328
397	330	275	321	342	310	257	365	382	358	271
323	351	316	308	402	319	110	395	368	396	220
283	401	371	329	384	369	353	379	374	353	301
286	334	312	414	397	336	405	282	324	372	347
351	122	301	284	431	403	251	298	112	303	293
305	273	304	290	83	226	313	329	267	100	370
392	347	200	298	490	433	439	268	288	568	209
325	320	415	279	281	355	304	443	437	249	457
621	195	791	999	330	366	379	477	388	238	370
383	413	190	228	423	160	283	309	382	319	269
337	0	328	238	405	292	412	371	383	457	4
236	162	453	420	303	405	187	356	458	397	396
231	268	303	330	355	336	329	46	322	369	302
255	409	433	175	275	291	312	337	154	118	408
265	319	466	311	317	277	349	266	345	137	372
0	368	194	409	347	385	342	204	352	361	411
345	340	354	368	305	323	248	318	398	405	278
323	34	326	331	314	460	258	398	419	320	311
226	316	449	322	339	358	287	357	253	353	462
256	246	302	358	352	307	472	326	104	314	296
273	337	73	405	288	102	403	161	395	393	315
254	265	324	319	302	333	279	337	303	279	



435

1459.3_1313EC36	340	286	169	469	399	318	415	291	347	394
263	304	272	364	220	255	395	224	3	341	377
559	217	326	371	260	245	294	569	280	925	288
257	254	204	226	343	144	320	374	429	486	234
244	314	323	443	226	250	418	246	288	312	268
537	372	377	380	488	264	372	270	352	274	256
273	324	285	257	293	275	298	275	218	305	356
227	196	335	190	215	240	230	227	186	328	324
332	314	368	308	345	240	264	300	288	335	301
335	268	253	173	280	168	255	299	425	321	322
277	256	256	306	595	275	307	192	233	183	246
269	320	281	293	312	241	284	282	313	284	258
270	278	279	285	527	337	178	659	328	385	155
274	304	234	281	243	223	253	272	270	287	229
233	254	209	271	273	276	267	231	285	269	283
298	150	175	236	281	266	246	213	30	224	223
157	47	214	229	111	256	275	266	241	113	443
235	113	63	301	338	415	389	305	246	330	70
220	107	275	127	170	283	312	245	538	185	321
191	289	295	330	999	213	387	438	64	227	205
508	284	230	231	362	271	240	289	311	450	228
130	0	217	180	392	400	566	275	165	393	123
339	186	399	215	267	342	230	394	147	344	300
213	68	150	265	205	338	257	177	278	320	313
269	282	348	166	235	143	362	161	153	171	428
144	115	322	199	358	1	337	261	325	156	316
5	164	219	222	404	139	272	226	305	613	373
217	296	303	335	147	224	289	197	284	284	224
322	10	212	296	257	301	334	250	329	233	274
341	193	380	274	253	269	131	197	294	209	219
149	173	322	305	288	243	347	315	94	130	192
222	243	54	235	252	175	246	68	296	288	266
181	232	239	265	239	240	176	203	213	265	

436

1464.2_1313EC75	330	318	205	282	347	284	301	289	453	250
315	285	355	404	581	705	298	358	641	365	313
297	193	364	269	347	468	370	309	472	317	523
488	549	443	545	438	228	439	269	337	291	281
302	310	530	281	182	368	333	223	366	314	425
302	328	330	332	305	251	328	317	333	283	306
291	402	340	311	257	396	288	340	568	364	281
373	424	307	395	448	490	199	304	452	353	362
366	386	382	352	374	236	418	414	416	384	353
387	428	374	271	368	231	401	181	285	407	404
289	349	353	331	298	312	233	446	254	448	389
292	254	153	381	365	338	194	158	299	296	354
253	247	271	210	302	188	264	332	247	248	248
247	149	338	345	334	317	336	338	333	422	356
396	318	307	327	306	312	326	305	321	308	330
358	273	170	305	321	307	240	390	190	375	382
264	300	318	348	307	84	328	315	308	296	318
513	577	173	217	259	301	479	326	199	372	43
362	690	438	365	467	388	379	415	307	287	270
338	137	332	366	213	999	331	291	529	169	483
170	446	216	323	385	0	291	226	439	295	153
486	0	463	279	267	258	334	299	424	357	40
165	154	264	462	259	429	186	308	462	396	412
181	425	312	338	332	240	354	59	409	273	383
140	443	419	298	339	414	138	472	187	140	403
394	431	305	211	217	295	395	226	295	225	238
0	369	0	384	270	575	362	219	380	339	387
367	435	240	343	383	261	239	244	242	391	398
321	149	350	358	348	427	177	463	413	302	317
201	264	408	390	333	407	255	345	301	330	479
374	387	395	369	362	298	429	331	159	384	306
334	315	75	403	320	141	318	236	357	366	324
322	323	333	357	276	372	317	327	224	305	

1467.9_1178EC16	378	371	286	386	370	353	443	218	289	341
381	263	394	487	348	344	396	309	306	401	323
389	295	302	440	340	326	389	371	349	434	317
348	328	293	273	264	249	359	374	395	425	341
343	445	357	306	180	348	449	236	347	444	273
291	293	288	274	467	465	280	346	264	303	301
332	313	306	304	321	371	420	302	322	265	438
241	334	535	274	283	384	221	277	356	282	266
280	266	268	288	291	275	306	305	309	330	268
343	299	281	306	290	208	283	373	484	360	354
199	212	218	238	304	273	285	346	263	338	271
254	286	179	286	267	257	222	380	280	415	247
256	293	334	240	504	426	297	420	294	273	264
269	458	302	293	307	311	291	333	327	330	304
292	340	347	353	342	371	341	300	323	333	327
369	293	225	291	346	328	233	257	109	319	247
186	150	312	263	313	201	326	266	316	279	358
374	313	191	361	320	443	291	212	289	323	236
378	281	255	257	301	316	117	302	399	287	318
351	407	349	379	387	331	999	410	311	211	268
472	268	631	232	365	315	314	355	319	292	196
256	0	326	342	564	401	299	416	219	321	62
310	148	462	243	364	329	279	439	251	314	433
232	232	234	374	271	474	248	309	274	424	315
288	363	386	94	251	217	484	287	253	269	343
340	222	294	229	443	239	265	192	235	43	321
2	246	90	227	468	334	240	224	241	341	403
240	294	444	320	407	286	341	301	410	301	258
275	26	335	317	252	360	325	415	355	289	311
245	277	399	262	222	298	198	263	210	248	322
218	244	400	296	341	282	353	338	142	286	280
323	322	98	319	322	103	276	115	356	340	298
367	297	347	354	332	301	151	319	248	236	

1474.4_1191EC10	346	407	205	411	400	410	466	242	364	421
451	400	405	453	273	321	450	254	237	408	420
454	342	363	545	291	322	406	451	349	474	325
329	324	238	248	288	129	325	506	425	366	304
238	470	314	350	186	320	393	302	323	413	292
381	299	310	297	341	459	293	340	275	335	349
334	300	363	347	366	322	386	333	278	264	370
307	266	599	276	253	347	246	322	294	308	286
310	311	318	319	331	238	317	369	319	336	321
349	303	286	175	299	137	299	391	429	334	329
191	229	223	252	435	324	319	295	281	292	219
263	288	216	310	259	225	266	396	266	418	251
299	365	293	242	355	463	186	334	300	287	251
265	481	283	292	305	296	273	323	307	356	304
280	262	229	308	293	283	294	241	282	292	297
271	144	319	259	322	298	235	185	4	184	257
243	22	211	190	162	245	347	246	267	89	384
355	264	157	441	395	466	379	230	372	431	446
337	272	287	232	289	320	155	357	477	262	426
350	315	400	477	438	291	410	999	232	68	258
307	337	251	251	422	7	249	407	301	392	209
268	0	304	359	569	337	398	377	245	347	32
286	153	468	249	331	313	287	356	279	304	401
265	191	181	373	314	513	285	287	308	360	248
345	356	317	160	217	262	573	254	178	244	438
213	229	334	313	451	175	292	313	297	200	301
6	252	136	263	409	249	227	182	251	431	393
215	274	456	323	272	342	364	339	425	313	229
371	139	324	311	266	420	371	350	441	339	379
224	322	464	288	213	313	237	248	246	251	385
255	205	334	321	317	338	355	267	107	236	245
214	329	212	259	274	143	304	161	318	293	219
255	250	385	378	399	381	222	351	377	282	

439

1476.2_1313EC75	311	267	136	347	363	284	322	275	485	276
329	286	309	438	630	630	361	425	597	389	369
321	236	351	275	264	460	379	268	416	282	463
427	416	947	536	389	171	315	272	401	274	363
342	349	448	332	109	488	454	200	285	234	422
310	265	276	280	317	318	271	308	306	307	355
300	399	367	373	279	356	261	359	479	391	303
356	387	302	464	386	474	153	364	448	448	381
388	415	364	362	422	178	397	428	390	402	406
402	403	405	179	407	131	414	215	260	423	434
302	327	339	318	345	334	267	443	215	442	341
348	244	182	367	350	332	104	232	323	331	341
210	212	282	262	230	120	184	279	247	258	200
186	135	386	351	398	369	379	421	343	399	380
377	354	347	404	395	361	399	318	382	387	419
360	170	162	347	376	378	247	367	168	370	368
311	339	342	329	138	160	281	295	323	216	332
410	497	104	189	254	322	467	188	252	308	187
293	610	403	282	513	338	370	474	316	314	106
346	30	273	388	64	529	311	232	999	306	566
241	511	228	289	402	0	331	255	402	336	160
456	0	463	322	311	296	334	333	388	348	0
2	102	318	514	263	388	58	288	415	344	414
225	460	361	282	392	224	406	3	367	287	444
49	400	422	354	314	336	166	470	30	12	460
320	394	446	196	179	335	336	302	241	145	317
0	367	1	324	221	473	331	318	369	347	371
327	414	246	322	333	135	165	194	276	363	404
131	254	292	348	343	377	47	386	348	180	92
199	179	372	412	307	406	292	339	278	380	438
353	348	376	329	304	375	382	320	218	405	340
325	359	0	348	342	56	353	201	358	347	324
266	360	237	187	221	277	241	280	191	224	

440

1481.5_1160EC15	226	166	20	151	246	5	143	34	188	138
183	334	188	216	266	260	152	249	168	165	185
85	74	223	179	174	188	193	275	248	262	240
193	204	230	291	225	6	219	61	117	276	211
237	220	300	169	0	219	195	147	38	139	229
173	140	202	192	134	197	165	146	189	110	89
141	143	200	93	14	216	193	106	214	152	487
197	202	101	153	253	198	127	17	213	145	185
206	138	156	207	176	192	200	274	201	217	140
285	208	218	156	181	168	181	107	161	261	227
250	217	217	260	146	183	127	167	143	167	197
185	64	165	178	160	182	0	141	123	187	142
176	33	94	23	78	43	143	206	132	67	81
107	96	138	141	81	161	95	98	52	245	189
218	198	125	229	249	117	212	197	170	205	169
81	155	0	273	210	211	95	174	94	121	160
9	5	94	227	173	146	156	134	258	162	217
178	199	203	2	4	143	300	0	149	257	191
229	309	249	223	252	195	325	305	216	4	7
227	142	239	238	227	169	211	68	306	999	252
242	293	6	189	243	0	236	27	164	167	1
300	0	300	217	183	140	238	111	217	222	49
129	0	187	182	126	167	240	191	322	193	221
0	199	191	146	312	201	190	236	189	466	278
4	172	159	6	330	226	145	173	4	111	136
144	291	59	36	98	29	245	6	212	0	90
0	160	0	213	153	265	223	155	194	250	184
186	161	89	131	189	106	160	5	31	144	180
8	3	163	163	171	159	1	198	173	121	17
54	5	165	168	335	185	161	134	150	6	288
218	199	196	214	192	118	140	267	2	204	169
198	166	0	139	273	0	324	0	207	169	226
163	308	110	153	205	236	4	161	2	1	

441

1488.2_1274EC17	342	246	96	334	339	316	364	276	506	261
383	324	346	399	573	523	317	510	498	414	348
372	249	430	317	261	482	383	309	506	321	515
500	488	521	967	566	77	481	345	464	274	418
314	309	511	324	120	442	424	292	319	285	551
292	524	536	542	334	333	545	325	506	309	410
305	522	452	421	291	357	267	441	440	330	284
397	401	316	438	414	482	184	361	465	474	484
518	478	505	347	498	182	468	494	467	539	467
538	474	477	71	475	157	482	263	279	569	564
372	474	480	505	342	415	222	496	316	502	402
450	237	269	481	432	437	216	269	385	406	483
332	304	261	308	295	171	67	314	242	244	173
283	197	341	394	370	335	346	363	357	437	367
416	383	420	448	451	405	416	416	493	401	490
404	55	215	440	417	424	204	404	280	437	423
406	353	444	455	62	267	308	467	351	59	342
516	511	102	219	295	364	523	255	93	380	179
343	493	491	288	573	407	267	576	412	370	260
390	84	359	370	205	483	268	258	566	252	999
199	588	120	274	446	65	327	274	462	318	150
507	0	416	321	298	282	292	286	453	558	36
181	106	358	519	296	538	138	357	523	546	465
190	379	356	237	374	244	366	161	456	334	482
177	449	492	383	435	390	224	456	209	62	542
333	485	430	247	213	302	566	350	516	195	330
349	419	108	485	202	530	481	205	513	310	495
435	500	217	444	376	204	116	249	331	428	522
354	94	342	452	452	440	267	485	474	229	224
219	225	487	448	368	431	247	363	407	354	503
346	397	402	410	379	401	402	445	299	365	380
409	370	138	396	447	203	344	48	425	405	386
301	341	258	281	254	308	222	334	279	204	

442

1495.6_1313EC36	267	247	34	275	185	272	308	231	277	219
213	288	260	299	139	256	300	161	125	396	250
376	166	306	317	266	264	316	283	325	497	316
303	279	219	202	250	20	252	292	291	560	136
135	283	325	192	250	208	390	183	274	270	218
224	173	205	202	471	279	184	243	243	196	247
277	242	298	246	245	184	287	286	183	201	352
182	168	303	184	152	247	176	161	168	198	139
142	204	205	359	182	66	237	268	232	189	204
188	209	130	126	129	61	170	201	361	213	183
151	205	205	236	219	214	389	188	257	186	185
158	300	117	201	241	235	203	179	86	314	157
222	213	208	130	655	309	136	518	318	292	124
190	298	187	186	238	222	240	249	277	241	172
160	193	164	241	192	163	210	179	188	175	204
198	142	246	175	223	186	117	65	2	100	90
84	2	112	84	20	225	222	101	184	60	253
265	211	43	336	297	308	338	253	234	287	3
287	257	207	209	166	404	0	311	378	219	361
248	222	304	383	508	170	472	307	241	242	199
999	224	356	403	330	511	131	223	292	240	186
231	0	246	8	321	400	287	222	224	238	203
356	66	349	257	281	285	120	443	286	256	247
167	217	134	262	222	297	293	231	156	360	154
171	250	201	201	249	209	298	236	206	82	306
195	252	187	284	328	0	178	282	183	135	255
0	148	210	241	347	267	222	86	226	281	249
212	241	297	228	150	256	210	242	282	256	164
296	9	184	239	179	203	267	272	284	266	312
249	239	222	169	230	148	148	217	134	240	261
231	195	219	237	219	234	322	254	6	212	162
226	183	98	161	209	163	248	96	249	233	217
151	214	236	246	243	259	166	237	232	251	



443

1503.9_1313EC75	350	310	58	350	360	323	358	272	729	316
336	327	316	408	512	485	325	421	456	377	417
393	264	523	295	271	485	370	322	621	385	574
617	607	556	607	904	0	799	409	374	283	367
359	355	658	329	174	397	348	290	316	326	558
322	702	687	694	274	359	697	362	738	271	555
334	821	590	573	252	391	319	598	401	377	333
443	553	289	478	394	547	240	448	514	702	782
781	726	799	305	786	166	709	738	711	792	712
794	693	715	75	730	179	721	261	318	776	775
343	658	664	715	342	507	193	575	307	584	562
513	244	308	676	636	493	262	258	431	439	547
306	327	295	356	250	181	78	273	272	268	203
305	177	440	537	472	449	456	524	471	518	436
492	572	486	668	680	504	644	541	708	625	731
511	0	306	632	612	620	246	450	207	422	461
379	370	415	460	0	269	363	455	508	0	386
459	469	66	139	294	358	745	234	91	380	132
302	481	535	229	458	356	398	483	389	337	229
344	76	324	413	284	446	268	337	511	293	588
224	999	124	250	316	215	366	264	611	349	218
492	0	518	311	322	300	358	344	768	768	0
209	199	407	496	321	726	195	426	642	808	594
338	423	264	256	464	248	419	118	623	292	697
126	638	723	431	630	371	226	490	232	148	670
273	759	613	305	221	292	767	440	745	190	631
357	591	102	621	242	485	732	194	746	359	710
707	742	224	676	359	253	197	325	322	641	629
439	161	413	615	653	750	437	587	693	286	243
189	316	636	576	635	617	277	455	652	537	720
504	428	604	638	629	565	499	610	362	526	467
573	472	244	539	586	95	604	232	626	625	623
315	481	290	292	283	334	245	400	319	282	

444

1509.3_1178EC16	223	142	178	301	304	155	217	186	99	205
266	144	195	227	191	164	323	198	118	257	223
203	188	150	182	206	101	193	257	166	239	224
161	155	203	108	84	183	87	248	289	253	157
228	185	171	233	49	213	240	103	233	214	123
248	136	147	147	280	294	151	247	248	222	230
251	249	220	229	264	336	196	238	250	201	256
174	193	293	181	187	233	169	132	247	175	225
193	128	180	188	237	160	150	105	148	191	162
191	149	174	200	175	79	177	181	251	231	232
160	87	87	87	218	145	197	233	166	225	60
151	189	205	191	163	113	134	250	165	309	213
115	123	263	229	260	240	240	316	212	203	192
115	212	240	221	235	241	214	239	211	173	226
215	214	241	202	202	209	205	181	176	202	166
227	177	50	179	201	196	166	230	0	241	243
190	0	247	235	149	187	191	170	192	176	283
242	305	46	241	181	217	80	169	76	193	4
202	197	110	107	37	268	4	131	169	69	144
210	35	151	190	230	216	631	251	228	6	120
356	124	999	237	246	45	181	136	79	235	3
271	0	215	165	322	248	231	223	63	146	1
128	5	295	207	230	74	81	313	13	221	303
32	17	21	165	1	210	86	106	75	235	145
180	246	161	61	1	130	226	137	98	138	123
29	1	175	34	181	59	118	178	199	1	202
0	161	0	6	211	274	99	0	112	220	230
98	120	178	201	258	158	58	170	235	179	184
62	0	41	187	178	36	243	89	141	145	203
67	166	180	189	7	187	67	159	190	205	152
61	205	247	129	124	202	125	186	17	21	176
187	224	0	205	186	92	205	0	204	183	181
243	188	202	175	179	152	51	199	15	154	

445

1514.1_1313EC36	238	185	55	285	335	205	221	240	239	200
326	184	295	281	319	291	229	239	254	544	308
230	130	203	312	140	248	243	216	225	289	226
236	218	310	254	247	42	241	283	347	283	343
358	265	281	190	138	339	368	166	228	223	342
165	205	197	208	278	342	195	221	238	207	227
237	253	200	229	235	254	174	192	286	257	402
263	263	254	261	209	305	127	260	288	292	223
260	292	244	515	282	181	255	265	262	313	278
312	265	254	59	261	129	256	245	394	294	271
183	216	219	219	190	243	325	277	156	273	247
222	280	165	269	265	245	82	213	263	263	268
167	170	223	208	324	268	64	224	287	256	116
156	209	210	243	213	219	213	259	236	240	298
248	255	285	238	211	266	232	247	230	214	240
219	67	7	247	199	193	199	186	192	183	224
234	248	190	221	54	148	160	246	199	27	313
305	310	131	183	234	221	258	191	110	240	106
170	307	261	182	186	583	237	228	243	43	182
231	142	214	228	231	323	232	251	289	189	274
403	250	237	999	318	7	400	370	291	200	95
203	0	225	269	231	368	134	288	305	224	28
160	168	357	216	251	233	156	165	236	258	275
241	313	226	175	201	213	249	174	229	365	279
123	264	276	263	229	222	181	274	25	105	326
228	259	231	15	278	233	271	192	244	4	194
0	205	0	208	325	292	263	176	250	147	247
284	292	210	245	243	96	158	42	192	237	225
193	20	185	235	252	270	123	236	306	113	128
211	41	366	241	211	284	190	233	215	216	258
310	196	251	318	323	262	143	216	133	242	271
259	254	1	218	216	82	201	0	235	261	243
225	249	100	130	71	113	155	155	125	75	

446

1520.6_1313EC75	344	320	131	390	368	359	398	263	417	333
306	362	426	549	353	391	393	246	318	519	450
425	182	388	412	282	391	489	409	389	432	408
377	377	358	433	341	118	312	343	986	383	318
285	373	363	388	178	366	368	301	325	346	322
407	290	295	312	400	496	297	276	280	231	409
263	308	422	401	275	294	364	425	353	284	324
245	364	380	235	308	349	210	309	298	347	294
298	326	278	469	319	176	324	340	314	318	322
320	316	300	86	306	146	298	314	425	360	329
247	281	300	307	496	312	331	278	269	278	272
264	283	193	256	281	237	207	332	334	392	231
267	380	287	238	342	327	87	407	396	345	181
245	324	265	266	283	277	271	284	274	308	255
231	273	259	327	316	301	315	254	296	307	300
302	114	225	295	318	315	216	316	110	337	327
338	304	296	330	116	218	288	273	262	113	372
376	358	15	358	365	398	424	243	241	395	196
385	343	309	229	320	457	355	420	427	271	283
379	222	387	423	362	385	365	422	402	243	446
330	316	246	318	999	0	274	289	326	416	165
283	0	298	305	423	306	439	370	343	322	11
117	128	518	404	347	274	171	403	369	316	352
246	339	285	269	344	345	314	241	389	308	329
223	361	328	250	285	342	332	339	168	60	432
325	334	310	271	332	361	273	292	235	94	231
6	291	211	317	365	372	296	245	293	481	328
294	311	352	338	343	237	292	260	409	312	276
309	169	318	287	272	343	240	344	367	253	260
314	252	349	290	285	285	239	267	266	241	337
337	280	263	309	305	290	359	313	151	313	240
289	260	123	348	276	181	289	224	340	321	300
248	258	230	228	206	301	220	254	235	215	

447

1522.3_1313EC36	273	223	1	127	119	99	142	145	110	164
134	76	174	82	118	69	184	105	0	180	0
169	25	3	59	78	14	160	118	114	301	1
97	105	0	107	139	1	44	153	124	781	37
74	222	8	70	164	110	208	167	203	213	120
157	115	69	58	292	0	60	175	58	143	21
175	59	109	21	191	105	222	11	114	136	152
126	0	249	109	109	144	205	32	30	211	60
26	27	62	0	26	233	23	13	20	117	28
107	24	16	192	15	166	140	203	282	96	97
115	41	47	56	156	32	202	69	218	69	16
28	64	178	62	61	4	115	236	102	194	83
147	112	60	169	413	225	219	426	48	53	13
112	224	137	157	192	213	147	163	163	145	170
146	13	30	20	139	194	17	10	133	125	118
126	231	5	35	15	97	123	26	0	65	53
66	0	58	56	3	35	96	142	37	1	155
0	3	43	15	0	142	148	170	145	114	0
172	2	2	0	1	0	0	3	215	1	59
0	23	190	160	271	0	315	7	0	0	65
511	215	45	7	0	999	0	8	138	0	165
0	0	1	0	188	319	174	4	0	55	10
142	0	178	0	177	4	0	111	2	3	135
2	1	158	79	0	305	2	8	32	177	2
61	28	73	3	1	0	271	0	57	2	48
0	1	134	5	299	1	28	246	32	2	8
0	23	149	4	343	25	199	0	3	127	27
2	4	297	25	0	16	10	14	194	1	6
2	2	272	60	3	36	18	10	55	14	26
59	14	62	62	3	24	157	1	15	80	1
2	58	24	105	53	218	13	4	0	79	19
3	115	2	0	103	175	1	0	20	1	4
110	3	180	102	64	36	5	121	163	32	

448

1529.0_1313EC75	272	208	269	281	253	254	217	254	351	235
238	229	278	362	319	301	277	275	373	269	250
214	203	339	252	315	263	315	226	273	273	288
260	255	315	329	310	271	344	284	176	254	405
974	314	391	188	182	429	478	176	250	261	312
248	209	214	192	198	261	189	234	297	173	217
230	317	257	216	209	213	260	236	285	283	624
279	217	252	263	278	317	184	261	304	291	241
256	289	258	229	271	195	323	277	332	242	301
263	306	305	243	247	131	280	206	548	260	262
257	272	272	271	234	230	195	272	219	267	300
219	247	163	279	298	295	136	175	170	260	237
231	187	250	253	230	267	210	257	248	208	195
233	324	229	210	262	257	245	284	283	354	241
245	237	277	267	251	239	251	224	253	258	271
261	174	103	230	263	234	193	170	158	149	160
201	223	160	166	208	98	241	231	239	204	285
335	255	139	263	272	217	356	266	246	238	106
315	300	300	255	320	310	244	269	251	195	268
294	274	257	283	240	291	314	249	331	236	327
131	366	181	400	274	0	999	347	372	178	98
305	0	378	197	250	464	251	282	354	256	157
209	70	286	250	171	256	348	289	296	324	269
244	363	226	244	302	244	298	209	255	609	285
173	341	278	258	251	301	234	317	175	236	354
224	333	305	158	426	239	297	306	226	143	231
0	235	0	316	533	400	327	247	333	264	274
282	328	272	294	274	208	330	211	197	288	226
238	74	254	301	263	313	269	353	304	214	261
197	223	266	273	195	233	201	275	219	280	331
302	262	285	448	441	282	317	261	224	290	279
292	264	126	261	240	81	240	7	277	300	248
271	249	242	270	222	250	195	219	191	206	

449

1538.2_1313EC36	258	282	144	283	351	284	377	178	283	344
282	251	507	328	227	253	423	209	252	299	233
280	203	301	510	305	335	461	288	260	331	263
290	308	222	209	298	99	253	512	239	250	401
354	462	306	222	225	333	437	230	348	522	281
248	216	226	223	252	291	220	288	254	262	203
315	268	201	204	289	233	491	194	251	221	395
222	199	406	229	212	276	169	323	225	278	247
281	296	251	236	286	221	247	264	249	252	283
235	235	240	68	233	182	235	464	543	253	247
225	206	204	218	224	269	257	227	220	224	230
214	238	173	248	247	253	186	479	299	277	234
212	256	241	165	249	478	60	185	284	250	169
201	457	222	260	222	241	202	268	248	264	283
199	215	275	229	225	211	225	191	227	238	245
229	60	158	184	228	207	165	190	73	183	191
175	217	181	208	53	200	262	219	199	61	296
291	258	77	493	255	377	270	162	311	290	169
460	216	254	215	248	279	204	294	306	307	389
247	346	250	309	289	226	355	407	255	27	274
223	264	136	370	289	8	347	999	355	207	93
235	0	266	316	295	460	247	280	259	278	99
264	60	329	246	306	247	381	289	241	246	309
140	310	303	276	248	511	309	333	221	400	264
399	321	273	145	202	260	379	293	190	159	345
184	279	294	181	565	121	232	223	193	113	273
0	192	156	220	561	266	225	70	233	235	253
225	265	522	236	232	224	327	195	407	233	221
220	13	528	257	221	362	360	377	423	236	269
232	186	479	204	264	252	209	211	209	211	364
267	187	228	343	332	296	342	226	199	228	274
241	260	90	228	206	213	243	76	249	262	230
258	241	230	252	221	277	210	257	234	204	

450

1544.5_1313EC75	338	326	80	367	364	273	343	228	582	239
341	395	306	408	514	454	331	290	427	360	310
484	261	466	282	277	434	341	333	577	397	602
560	555	417	441	587	56	556	339	337	333	320
353	344	889	366	223	403	379	255	325	306	637
304	484	461	466	315	311	460	300	560	255	416
246	584	443	423	259	320	334	449	348	343	305
323	402	361	350	363	442	199	384	377	489	499
491	476	500	332	493	143	532	504	512	605	496
620	525	514	96	501	147	508	269	346	590	568
316	511	498	545	314	407	254	465	283	463	575
471	290	210	673	624	503	219	287	300	342	430
263	301	306	283	320	182	96	294	295	326	153
272	223	311	362	352	315	312	381	378	399	419
347	426	338	488	485	336	454	391	536	439	547
334	28	256	485	438	425	225	337	105	378	346
324	246	331	351	28	245	254	368	357	32	362
423	384	108	253	254	343	589	187	127	452	215
327	385	654	264	440	327	325	410	467	490	265
319	108	328	382	311	439	319	301	402	164	462
292	611	79	291	326	138	372	355	999	376	214
384	244	383	296	331	270	296	403	532	519	0
188	79	343	463	278	512	98	352	482	574	398
293	408	383	295	369	285	310	58	476	252	744
160	402	498	386	401	329	242	394	137	2	463
256	496	433	257	299	341	512	268	499	26	484
7	442	129	454	292	412	565	271	549	333	524
439	683	289	521	318	238	212	235	312	520	494
331	103	373	470	487	573	300	452	508	298	237
197	228	457	522	475	428	275	347	438	370	586
376	340	404	485	453	394	384	428	289	423	343
407	329	186	412	418	37	422	82	447	443	436
285	376	200	216	188	248	226	277	219	211	



1560.7_1191EC08	292	245	210	424	338	332	389	182	413	332
218	324	308	386	281	369	376	276	355	379	562
520	207	366	472	244	295	330	624	285	540	261
284	284	311	333	373	175	325	362	457	316	224
182	317	473	900	99	306	323	266	257	310	291
552	310	320	305	352	385	304	208	327	240	320
219	334	304	317	215	256	275	319	302	274	293
267	316	300	259	298	322	231	246	285	302	293
313	307	332	260	304	221	286	323	294	358	302
357	271	292	109	282	132	303	297	364	363	369
240	289	289	316	667	239	185	273	265	270	261
220	188	193	305	293	236	202	266	282	332	273
266	291	254	289	297	271	108	529	263	316	150
284	289	259	270	260	246	261	300	284	309	258
276	281	265	312	309	300	316	287	325	319	313
297	132	204	285	308	309	181	266	79	261	261
261	132	270	241	165	205	240	309	276	132	391
360	321	16	236	375	389	416	181	274	375	91
358	340	296	183	331	340	420	308	517	237	222
362	168	334	319	450	295	292	392	336	167	318
240	349	235	200	416	0	178	207	376	999	149
262	0	288	201	323	271	537	251	365	347	174
76	3	414	293	293	376	156	356	321	337	374
201	294	268	221	220	298	273	65	374	279	299
207	294	296	263	281	300	318	337	151	12	431
216	331	251	245	279	287	313	263	320	149	378
4	264	47	267	309	390	294	380	304	623	377
286	325	298	494	228	170	156	226	288	493	280
287	188	217	255	292	346	251	370	364	230	210
288	223	349	303	262	277	196	258	305	218	270
272	273	296	307	254	296	313	307	91	322	253
305	247	11	307	287	168	297	203	296	315	277
185	258	147	172	206	227	115	165	161	183	

1565.1_1274EC17	203	363	13	199	162	248	176	84	234	20
153	335	144	203	221	243	110	136	247	230	198
184	270	218	142	230	211	206	220	253	244	248
244	254	185	185	245	237	256	210	147	238	149
195	173	199	146	929	236	174	255	238	199	200
313	256	240	235	180	176	219	125	226	142	141
133	210	203	150	111	156	155	154	167	175	175
147	254	210	153	261	188	215	125	229	215	194
200	193	195	146	204	109	223	283	202	191	186
184	194	176	14	177	111	211	201	190	230	227
218	203	203	216	234	151	277	179	216	179	155
121	185	185	190	186	148	243	186	190	203	131
246	287	182	160	200	193	126	176	226	164	156
248	172	149	185	120	148	133	164	153	215	205
174	172	220	280	268	130	229	200	260	277	248
139	196	151	243	251	263	126	207	72	231	199
30	17	154	189	8	60	229	175	233	0	202
214	194	139	100	207	176	270	63	85	322	2
167	159	199	98	189	152	295	205	192	142	315
170	175	255	269	228	153	196	209	160	1	150
186	218	3	95	165	165	98	93	214	149	999
126	0	190	126	239	148	282	141	300	240	0
244	5	173	140	32	230	130	184	219	256	233
130	151	159	120	177	231	139	1	150	178	173
208	220	204	7	228	166	171	164	139	0	227
141	273	223	179	194	83	226	239	218	81	232
15	216	220	229	178	206	226	57	236	209	240
265	211	158	276	205	190	195	151	182	267	137
154	3	154	224	218	239	138	184	211	185	170
125	183	239	226	306	182	114	94	137	144	174
227	159	169	182	189	166	246	213	64	209	157
229	164	30	287	214	77	285	99	283	262	272
150	168	201	240	198	259	182	223	252	226	

1573.9_1274EC17	239	249	125	283	302	226	239	295	404	238
315	271	274	332	474	420	247	377	481	341	237
267	251	355	215	269	371	275	210	325	261	423
359	423	476	494	415	178	425	308	284	224	322
292	308	445	240	172	380	266	290	333	215	463
229	345	349	354	245	318	353	300	382	270	334
282	393	351	352	272	381	226	368	441	321	272
357	297	245	458	325	489	199	404	429	431	377
360	400	397	276	431	213	396	410	397	462	419
461	394	405	140	424	195	413	210	262	468	468
282	400	404	420	227	412	142	472	211	468	404
356	198	204	454	420	393	129	187	283	315	512
200	257	258	289	234	172	118	187	276	220	293
194	159	311	361	332	319	308	363	343	357	363
402	377	299	408	423	354	400	409	428	397	435
345	169	209	421	392	408	239	395	184	389	401
412	336	360	395	136	231	338	411	340	182	288
358	392	138	186	232	239	430	239	98	357	231
313	393	377	242	462	345	236	509	272	342	154
346	105	222	337	130	486	256	268	456	300	507
231	492	271	203	283	0	305	235	384	262	126
999	1	708	294	264	195	259	338	361	375	99
225	181	314	468	417	475	197	273	396	421	424
283	378	284	252	474	166	356	90	444	244	431
163	502	531	279	440	312	114	460	250	184	473
300	496	400	201	153	255	413	298	359	203	321
424	384	0	354	200	494	408	215	423	245	419
421	437	203	356	345	180	114	203	258	324	528
273	100	279	407	359	491	141	462	399	203	179
242	213	400	384	324	398	296	316	438	369	437
324	381	462	437	406	345	357	433	290	399	453
408	386	168	350	439	89	359	44	398	427	421
280	322	270	257	236	294	196	317	223	242	

1580.7_1313EC75	0	161	0	0	0	0	0	148	1	0
0	0	0	0	0	0	0	0	0	134	0
0	0	1	0	106	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	228	0
0	0	0	0	0	136	0	215	237	0	0
3	1	0	0	0	0	0	157	0	177	0
156	0	0	0	195	109	0	0	0	241	0
204	110	0	0	160	118	264	0	6	118	0
0	0	0	0	0	170	0	0	0	0	0
2	0	0	129	0	168	0	309	0	2	2
301	0	0	0	356	0	0	0	262	0	0
0	0	158	0	0	0	224	29	480	0	4
240	125	146	208	0	0	130	0	102	0	0
175	0	175	185	158	149	160	172	181	139	152
101	0	304	104	104	152	104	1	134	146	126
261	106	0	0	0	0	253	7	0	20	133
5	2	138	5	107	1	114	15	90	80	0
0	142	497	0	0	0	0	154	0	0	0
0	0	5	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	244	0	0
1	999	0	0	0	0	2	186	0	0	1
3	124	0	0	0	0	0	0	0	0	174
0	0	0	0	128	0	182	0	0	0	0
0	179	0	0	1	218	0	0	184	0	0
172	1	0	0	0	1	0	0	0	0	0
1	0	689	0	3	137	0	196	0	338	0
1	0	0	0	8	88	155	0	0	0	2
0	0	0	116	0	194	0	0	0	147	2
0	0	0	1	0	173	12	183	71	214	0
0	1	0	141	132	1	0	0	0	3	1
1	98	177	0	3	0	0	0	0	0	0
122	0	129	50	81	0	0	5	0	158	

455

1581.5_1274EC17	257	217	96	324	339	213	265	240	445	271
316	243	269	322	445	445	309	324	433	335	252
305	282	363	216	281	477	293	237	321	296	350
343	352	502	402	454	90	427	320	280	242	373
354	299	399	256	236	434	359	252	296	249	384
248	392	399	401	236	348	399	307	415	220	355
301	430	372	362	237	363	294	377	402	332	283
283	336	243	476	273	548	216	408	423	477	401
414	444	395	246	402	156	408	409	426	490	523
487	407	393	123	410	189	416	221	289	471	470
309	430	434	464	252	374	165	414	234	420	415
333	254	228	461	444	354	199	263	257	401	428
255	261	297	281	242	145	119	216	274	288	241
256	162	334	371	380	376	353	422	408	447	367
344	355	376	406	407	388	401	312	456	400	449
370	86	280	390	398	395	282	333	177	337	341
333	321	347	323	72	192	343	329	390	82	326
371	355	151	181	214	265	444	195	140	293	211
284	434	352	238	430	283	249	446	331	304	230
277	80	227	328	217	463	326	304	463	300	416
246	518	215	225	298	1	378	266	383	288	190
708	0	999	290	251	239	262	293	414	417	116
164	167	348	473	389	509	199	350	396	450	445
269	424	254	270	371	190	351	97	446	243	423
154	422	494	347	360	271	140	508	131	193	465
281	438	431	290	180	238	440	236	358	156	401
6	374	136	373	208	477	450	170	459	276	442
391	477	174	424	341	262	123	307	287	391	457
320	85	306	394	391	472	173	416	436	274	276
177	312	351	385	366	377	222	351	413	361	423
331	350	478	415	390	379	386	399	264	364	396
349	359	141	342	394	94	349	222	385	399	370
307	332	342	348	362	371	288	373	292	280	

456

1595.8_1274EC17	195	211	145	185	200	180	235	246	272	180
639	152	241	426	310	339	253	230	306	262	236
221	164	243	279	287	335	295	222	291	238	289
308	287	226	314	247	201	298	350	269	207	305
240	349	287	221	163	347	295	137	184	236	265
158	232	260	234	161	287	244	281	240	306	231
277	284	258	231	330	212	250	237	265	271	261
207	261	479	226	226	312	160	226	263	339	226
228	306	229	234	246	196	230	287	237	273	333
271	213	175	183	186	194	212	159	281	278	279
165	256	256	238	203	232	175	281	223	275	252
212	235	158	275	254	266	129	178	196	300	247
167	199	267	183	173	297	221	246	227	236	242
183	281	224	222	235	229	190	229	232	304	180
221	252	245	268	268	208	269	225	260	267	300
237	228	63	243	261	254	155	193	164	171	199
190	157	174	198	157	179	279	257	235	161	174
318	291	113	230	198	235	284	264	121	229	610
277	349	239	286	298	261	210	311	205	271	177
271	188	198	238	180	279	342	359	322	217	321
8	311	165	269	305	0	197	316	296	201	126
294	0	290	999	475	190	161	384	279	298	67
119	2	257	233	237	307	210	259	288	281	261
227	331	247	284	301	466	289	9	324	238	303
209	335	300	354	253	322	462	264	134	310	305
275	302	241	184	244	193	237	267	213	0	237
0	246	0	232	233	333	248	235	285	227	297
288	317	342	296	215	179	263	175	232	227	278
234	85	175	254	231	284	158	295	324	189	211
197	178	311	220	232	182	213	221	274	206	320
234	275	285	340	382	240	249	259	205	330	234
295	269	218	228	227	197	200	0	258	248	276
224	276	229	250	213	260	200	248	218	172	

1623.5_1313EC36	332	406	206	482	457	367	420	179	316	312
647	347	302	584	346	315	378	289	283	358	412
411	301	322	386	299	309	366	439	367	451	336
361	337	305	291	334	202	399	437	430	343	348
297	383	325	300	216	370	358	266	356	344	306
368	291	331	315	365	450	321	312	332	303	347
293	312	325	349	307	323	354	313	251	231	372
217	330	658	273	278	358	248	284	319	334	292
298	306	300	336	307	214	342	398	335	364	304
371	324	304	216	309	193	310	271	417	388	380
239	273	274	287	371	318	278	338	291	339	266
274	294	223	296	310	252	274	269	274	446	267
285	319	285	246	416	408	225	371	290	301	233
294	440	275	265	283	289	268	312	331	342	270
248	312	286	382	387	298	365	300	376	373	380
303	208	248	339	378	365	240	231	91	237	255
237	152	237	203	208	212	351	258	326	173	456
376	303	79	255	344	420	359	160	287	378	593
263	277	287	216	294	293	321	315	413	240	307
254	282	354	405	392	267	564	569	311	183	298
321	322	322	231	423	188	250	295	331	323	239
264	0	251	475	999	346	366	457	316	342	55
233	143	463	301	381	407	186	391	264	370	385
293	188	217	338	356	514	224	222	322	370	243
210	352	377	192	339	196	614	231	224	303	456
255	313	344	265	376	185	307	356	296	119	367
28	276	70	280	365	322	277	205	305	344	461
315	296	393	413	344	286	334	285	347	398	283
298	35	279	351	304	414	252	342	424	296	320
239	282	429	323	380	297	209	269	268	281	392
292	189	384	378	371	298	358	359	144	258	286
344	293	164	358	343	128	365	98	378	357	349
302	281	332	334	326	330	135	308	273	276	

1625.9_1274EC17	282	267	168	403	378	221	303	195	282	288
288	284	377	359	286	306	333	342	255	331	379
370	196	269	326	302	225	376	312	273	437	270
281	262	340	286	258	171	299	330	301	375	395
458	436	284	271	167	391	927	193	286	355	262
332	233	239	240	376	283	235	269	260	193	240
260	216	232	239	246	270	332	228	235	200	427
174	271	357	291	244	327	184	333	226	289	217
240	240	214	287	254	188	261	301	253	319	240
322	240	245	218	258	119	246	292	516	340	333
232	259	257	230	319	243	272	210	211	204	230
231	290	188	235	249	199	194	253	234	337	243
220	237	293	233	399	350	209	384	313	296	150
227	309	231	276	243	254	228	277	282	313	260
275	225	348	293	294	330	278	203	278	291	284
354	156	203	258	285	269	200	211	125	207	224
176	140	189	199	184	197	270	250	233	161	381
301	239	154	280	251	303	315	144	246	290	153
336	302	230	205	367	261	357	273	387	166	275
226	258	253	292	400	258	401	337	296	140	282
400	300	248	368	306	319	464	460	270	271	148
195	0	239	190	346	999	341	300	270	240	134
215	124	310	268	303	302	278	376	310	282	261
253	215	227	248	201	352	215	272	207	450	242
221	295	304	154	247	198	312	232	194	213	423
179	258	291	193	445	160	270	222	226	179	301
11	264	108	225	485	279	236	172	253	322	337
289	252	333	321	254	234	307	198	316	312	250
285	34	313	316	264	327	274	307	316	246	280
255	193	354	317	301	254	201	215	238	235	258
270	258	246	330	335	278	326	257	242	196	260
224	235	38	258	249	44	265	166	280	277	303
257	220	263	285	246	279	137	246	231	188	



1640.8_1313EC36	322	357	137	455	362	315	389	223	455	356
252	371	294	382	316	365	361	247	331	350	521
480	205	433	334	276	309	386	636	382	598	344
369	346	290	335	371	163	333	323	485	401	240
244	356	386	546	290	340	376	337	336	303	332
969	362	349	344	426	353	337	253	362	253	328
265	386	344	329	256	311	317	329	291	305	336
264	302	322	245	363	311	368	289	303	363	332
339	338	352	302	320	276	317	345	350	370	337
367	328	314	191	336	334	336	299	318	369	367
302	303	305	341	737	294	204	253	304	251	276
248	228	257	344	321	258	336	297	341	306	309
327	277	289	286	350	234	196	564	266	356	160
347	225	283	293	304	279	279	316	288	319	254
317	300	262	352	350	378	367	341	360	358	343
302	161	193	308	378	353	215	265	80	271	276
273	175	260	256	139	233	309	306	288	127	457
379	350	137	207	326	389	458	246	239	409	10
309	272	302	260	325	280	469	313	558	199	210
311	167	333	412	566	334	299	398	334	238	292
287	358	231	134	439	174	251	247	296	537	282
259	2	262	161	366	341	999	334	349	393	0
173	74	396	264	256	364	151	345	346	371	355
159	293	231	262	288	271	298	11	404	292	301
194	352	346	243	357	307	281	288	233	5	449
157	364	357	209	274	241	346	241	331	267	290
145	282	264	292	324	353	315	332	333	709	384
340	354	272	364	337	243	175	204	311	378	306
343	152	275	300	290	396	256	315	362	254	266
265	216	338	320	326	289	181	228	321	238	313
247	251	328	324	271	324	367	348	234	277	257
310	288	76	360	351	119	363	28	366	374	327
230	250	256	256	244	315	248	280	263	240	

460

1653.8_1191EC10	306	344	123	335	332	251	296	178	238	269
352	300	340	389	314	390	292	266	324	390	269
304	187	297	344	296	315	407	339	356	339	330
360	335	279	253	256	84	327	310	324	321	326
272	431	381	268	174	389	320	226	284	445	352
285	302	318	314	284	313	307	370	309	417	288
370	311	315	305	403	336	395	277	267	309	348
352	218	478	299	273	388	192	341	292	327	290
311	291	321	378	328	161	337	307	356	319	312
339	328	296	163	288	157	298	276	403	351	346
209	284	285	297	299	282	201	270	247	272	286
253	283	205	303	263	236	138	258	223	321	295
253	286	255	202	359	534	139	303	335	335	177
180	364	383	479	384	393	351	377	394	407	358
333	323	274	335	326	251	338	314	298	340	301
278	110	113	303	350	335	174	193	27	199	191
162	235	136	252	175	198	356	229	310	114	329
344	303	160	360	264	296	266	196	232	328	285
377	352	318	307	255	389	203	248	327	300	280
360	268	340	371	275	299	416	377	333	111	286
222	344	223	288	370	4	282	280	403	251	141
338	186	293	384	457	300	334	999	343	359	128
307	103	333	284	287	337	239	346	359	340	397
320	291	259	264	323	462	364	333	363	346	366
215	377	314	316	297	398	440	268	228	187	325
244	355	340	115	458	142	319	197	291	150	247
0	290	226	305	421	382	292	226	329	347	352
327	339	408	347	406	284	435	188	367	308	316
532	381	325	308	297	474	262	342	437	270	250
274	188	383	332	283	472	283	368	277	341	390
377	375	315	341	315	389	331	350	208	322	465
374	445	392	278	311	89	331	185	373	376	317
427	469	328	331	304	374	209	345	302	206	

461

1659.6_1313EC75	322	274	1	308	353	247	328	269	664	215
330	397	330	360	422	462	296	280	412	419	522
399	174	452	255	202	443	316	276	622	343	586
617	619	418	460	745	0	639	358	409	268	348
324	369	593	345	216	390	351	231	321	302	479
339	545	544	549	297	320	555	286	609	253	506
286	677	539	518	240	333	255	550	398	368	330
330	680	221	440	323	482	189	340	524	673	636
641	683	625	362	639	139	611	695	623	609	665
608	609	637	65	652	118	642	229	298	638	638
309	570	572	594	302	420	263	505	258	507	475
430	305	289	529	531	404	169	235	361	372	451
257	247	241	335	239	194	58	271	349	329	130
208	163	391	470	412	400	404	466	424	463	374
469	498	425	629	658	408	608	466	664	608	655
419	0	285	597	573	587	224	453	137	399	462
379	395	376	454	0	227	245	418	468	0	376
399	465	144	130	269	328	669	113	140	377	20
282	411	525	257	274	345	516	400	391	227	199
316	118	282	383	165	424	219	245	388	217	453
224	768	63	305	343	0	354	259	532	365	300
361	0	414	279	316	270	349	343	999	606	0
136	59	379	398	246	546	171	299	575	680	518
291	393	387	243	393	224	380	63	477	289	510
122	561	557	405	632	295	170	411	162	83	580
289	723	514	254	145	325	622	517	582	52	483
140	488	173	534	196	505	642	267	650	317	615
709	638	191	691	343	257	153	260	287	696	511
212	211	333	540	587	655	404	469	565	279	236
266	249	589	562	722	535	290	409	437	427	613
506	412	442	518	514	489	420	511	263	453	445
467	433	167	605	490	116	617	179	576	622	657
267	440	218	200	166	262	146	302	186	259	

462

1670.8_1313EC75	354	315	193	360	338	354	338	232	582	290
317	326	357	406	383	435	327	350	350	362	356
461	265	474	353	289	424	365	345	536	491	492
528	517	390	552	808	236	715	407	373	307	333
279	342	538	332	200	344	293	222	328	294	515
385	931	949	947	368	318	932	317	780	270	528
322	772	540	531	289	347	289	553	377	378	302
368	412	301	404	344	430	202	390	445	647	915
911	697	906	284	889	156	619	581	638	760	671
795	620	650	208	672	127	660	240	282	701	702
323	649	660	774	367	510	225	449	297	447	488
480	234	284	590	590	441	311	245	321	419	601
353	365	219	339	329	279	183	376	267	250	165
327	291	431	498	448	425	429	479	438	450	406
448	547	440	581	587	421	573	493	667	574	684
454	201	297	578	567	576	176	419	229	461	423
425	394	430	470	196	316	322	459	452	201	363
421	377	96	257	346	338	624	209	216	356	164
324	408	539	277	369	369	339	444	455	278	304
351	249	354	457	393	357	321	347	348	222	558
238	768	146	224	322	55	256	278	519	347	240
375	0	417	298	342	240	393	359	606	999	1
296	153	390	421	327	679	252	441	612	799	568
312	336	268	267	406	267	402	206	593	296	641
220	539	595	429	497	285	244	394	250	165	646
285	619	606	301	256	335	910	362	868	166	599
394	584	148	622	255	373	684	207	698	377	687
574	630	273	543	293	289	280	317	248	522	598
479	268	340	572	604	623	420	511	652	306	315
223	286	671	484	554	569	300	419	662	452	628
387	358	599	585	552	498	459	600	312	537	432
503	457	173	420	540	202	521	240	590	576	555
282	432	289	348	305	359	247	358	332	341	

463

1673.2_1313EC36	51	142	85	72	160	50	30	90	45	50
140	154	19	58	82	0	60	97	80	84	185
46	37	25	42	24	65	105	214	26	194	0
25	21	24	46	36	65	195	27	150	8	202
123	175	0	133	0	371	44	136	178	155	21
46	29	27	29	160	109	27	133	44	46	27
114	47	29	27	61	186	29	23	156	43	173
52	181	116	42	55	194	37	160	164	227	33
39	246	118	151	144	24	28	109	24	212	247
154	28	32	47	33	12	29	25	195	136	159
240	31	13	37	83	23	161	80	34	80	24
16	187	27	41	41	0	1	0	26	123	95
22	135	23	162	63	140	46	2	164	184	61
155	194	44	165	149	137	101	136	79	137	180
195	94	78	53	45	56	53	75	22	137	122
21	43	3	61	40	35	29	1	170	236	128
0	0	203	156	42	88	100	171	159	88	119
1	213	1	1	44	30	33	0	56	4	79
0	0	76	16	71	37	0	0	41	0	93
87	147	54	4	123	40	62	32	0	49	36
203	0	1	28	11	10	157	99	0	174	0
99	1	116	67	55	134	0	128	0	1	999
220	70	106	2	0	22	149	59	0	65	42
202	3	0	54	89	152	23	126	1	141	0
1	134	0	0	0	164	143	0	121	26	88
87	0	7	62	179	103	0	160	41	2	40
0	32	0	0	184	257	38	62	47	205	60
0	1	155	34	3	156	214	52	7	0	0
2	0	0	134	22	0	0	316	3	79	105
227	55	12	104	0	60	119	43	83	1	0
0	0	165	119	203	46	63	150	68	47	95
0	173	0	2	102	0	0	2	37	0	140
109	0	92	86	38	22	0	44	32	5	

464

1673.8_1191EC10	257	291	118	316	296	210	252	245	199	204
306	196	134	253	260	269	218	249	157	279	189
283	249	260	200	199	259	174	232	271	363	226
260	209	217	210	206	172	240	296	245	301	277
287	229	248	151	227	361	297	253	332	255	184
237	300	296	290	503	212	302	305	206	246	248
305	220	281	249	268	308	242	257	270	237	349
200	276	324	249	274	321	235	277	270	325	231
276	269	242	103	274	182	314	230	317	243	271
273	301	293	187	314	232	311	216	336	268	275
260	242	235	221	258	289	309	289	282	314	177
288	344	294	224	214	242	228	213	304	264	219
277	319	244	272	375	297	221	220	338	281	179
248	250	258	345	298	296	298	346	336	351	293
291	245	240	270	262	301	274	221	293	267	268
282	184	115	260	251	260	222	295	152	222	312
148	3	291	190	190	213	291	318	268	145	284
179	279	276	133	221	252	240	209	114	184	103
95	115	240	24	146	100	0	180	231	2	338
96	117	209	236	339	165	310	286	2	129	181
356	209	128	160	117	142	209	264	188	76	244
225	3	164	119	233	215	173	307	136	296	220
999	155	248	134	217	200	164	239	151	234	326
95	8	173	284	174	216	148	179	118	270	252
187	367	172	49	102	156	228	125	184	150	279
224	7	295	223	257	212	245	192	263	139	254
0	296	201	215	293	174	224	80	267	271	277
218	222	206	275	172	285	115	241	179	208	117
118	93	92	342	302	237	249	120	339	272	219
180	251	334	231	214	313	159	163	164	256	150
56	240	243	373	365	243	235	241	31	243	225
93	294	122	186	258	107	141	225	221	220	199
251	122	329	304	266	261	275	264	225	242	

465

1675.0_1274EC11	129	172	139	75	77	115	87	421	175	44
266	111	170	188	137	126	105	180	313	160	43
90	91	128	135	110	111	210	91	120	98	148
122	126	115	100	178	169	235	110	57	73	51
93	137	72	48	160	191	92	123	94	102	103
75	164	169	166	153	89	165	353	164	287	130
303	153	109	127	305	369	93	109	164	320	137
346	207	75	117	215	181	96	121	174	200	172
175	145	168	43	198	103	124	197	118	157	189
165	117	101	125	122	203	121	213	108	177	176
183	167	170	185	135	128	0	170	145	170	141
137	146	219	147	105	130	191	114	237	144	188
170	135	252	243	97	78	136	94	264	77	138
158	140	262	346	257	294	266	274	354	380	302
274	136	88	160	177	271	143	179	200	209	235
232	162	227	165	143	168	301	191	104	211	222
239	69	189	113	149	237	215	212	193	117	44
158	78	192	114	82	87	165	426	2	98	248
172	148	102	92	154	166	11	154	131	55	158
1	225	81	162	186	154	148	153	102	0	106
66	199	5	168	128	0	70	60	79	3	5
181	124	167	2	143	124	74	103	59	153	70
155	999	122	92	154	225	152	200	134	174	282
176	75	167	191	46	103	344	0	149	84	145
225	155	141	149	252	292	110	168	166	139	136
103	236	127	210	2	79	187	242	147	168	76
205	178	135	146	76	97	143	136	151	100	138
225	162	114	169	234	157	92	172	119	121	239
278	220	93	225	186	69	72	139	153	142	117
0	214	88	124	244	262	319	276	174	269	160
243	280	195	146	142	263	222	185	214	281	209
190	279	328	82	183	82	168	126	143	158	195
268	201	227	232	165	177	85	213	175	161	

466

1682.1_1160EC15	552	336	174	411	333	589	364	198	379	324
298	394	379	415	272	343	345	240	309	533	531
471	274	326	562	269	346	394	449	336	460	348
342	359	334	345	434	146	428	550	506	356	403
301	331	328	417	206	327	362	265	301	339	345
370	343	337	348	362	960	339	288	348	233	367
284	352	362	376	258	306	335	353	349	262	376
241	334	393	297	273	390	201	338	320	362	364
371	340	381	564	372	220	355	402	344	404	330
405	342	337	151	356	190	343	288	394	415	411
224	316	327	365	396	339	326	315	238	313	293
306	309	169	319	321	273	244	225	309	458	315
275	378	327	242	401	409	152	407	398	382	165
266	412	289	322	300	300	290	343	332	353	303
255	292	349	388	370	323	357	295	372	332	354
302	159	322	348	367	361	218	244	98	258	256
201	220	253	200	154	187	326	278	295	161	380
428	413	101	268	607	364	420	148	226	398	197
266	314	326	178	268	451	421	395	427	245	396
499	236	431	453	399	264	462	468	318	187	358
349	407	295	357	518	178	286	329	343	414	173
314	0	348	257	463	310	396	333	379	390	106
248	122	999	360	349	392	185	340	354	388	426
241	236	199	337	431	365	267	159	331	349	349
210	451	449	200	311	251	339	322	223	181	540
206	343	331	320	324	185	369	283	365	70	370
11	260	146	302	366	296	361	215	377	389	411
331	343	343	373	346	305	315	327	352	366	313
287	38	320	350	318	394	271	387	397	282	274
359	331	460	341	375	343	222	269	291	267	391
269	207	390	360	342	320	401	369	208	297	328
321	301	96	341	341	127	348	173	415	360	343
291	266	293	311	235	305	175	309	274	212	



467

1694.8_1313EC75	334	287	0	279	345	294	341	267	460	260
289	377	361	384	496	451	374	288	459	382	336
371	135	458	280	223	368	370	289	468	341	453
471	466	503	475	470	0	383	319	437	264	409
271	269	535	271	145	426	440	252	320	242	438
271	350	345	348	342	364	342	272	376	253	429
263	440	436	435	211	265	262	439	451	283	272
324	384	297	386	335	475	167	374	444	445	436
443	425	396	286	450	143	396	395	398	509	451
516	394	408	179	416	250	411	238	281	505	507
319	367	369	378	330	345	209	549	169	547	334
358	241	141	465	417	355	152	286	325	378	368
170	165	284	230	265	221	144	243	319	289	171
219	164	322	372	340	328	320	374	353	391	370
334	389	384	409	406	366	397	327	400	383	386
347	0	185	365	368	381	268	317	213	350	335
266	249	312	324	0	148	286	302	319	0	314
390	458	2	152	262	341	452	112	173	450	25
296	443	483	226	373	265	252	450	362	273	145
335	15	359	420	215	462	243	249	514	182	519
257	496	207	216	404	0	250	246	463	293	140
468	0	473	233	301	268	264	284	398	421	2
134	92	360	999	249	484	0	319	525	425	427
215	365	292	228	432	252	270	177	358	249	497
250	439	560	258	313	350	172	432	7	1	474
238	396	371	109	206	261	430	242	390	0	358
8	321	0	334	233	435	391	246	441	317	440
328	460	279	349	269	157	160	131	375	322	390
291	292	364	364	383	492	243	406	411	195	143
188	131	415	389	338	424	246	330	384	296	477
324	300	377	403	351	317	312	357	273	351	404
322	272	7	341	356	1	303	10	398	372	297
280	326	220	108	27	193	52	175	116	193	

468

1708.2_1313EC36	277	264	49	344	338	281	314	164	252	296
324	209	307	344	363	305	297	349	313	293	286
318	214	337	362	235	313	331	292	336	345	334
311	272	263	324	285	44	270	355	375	317	181
204	365	236	244	119	440	271	241	265	345	255
278	289	326	290	281	311	321	289	270	228	248
301	268	276	253	257	338	310	261	317	197	353
231	196	377	316	308	381	219	201	290	318	271
277	277	290	276	306	130	304	318	303	324	271
342	291	301	77	284	161	264	279	302	341	341
256	279	278	259	299	295	243	317	239	317	215
232	268	226	218	207	234	203	275	170	349	252
236	259	254	286	365	279	83	340	319	248	161
225	302	227	316	272	299	218	295	299	334	295
261	279	237	331	314	270	312	251	330	316	368
244	87	184	246	324	332	232	282	201	212	295
246	210	262	209	53	188	295	302	251	46	355
337	371	208	277	244	314	281	157	279	271	272
362	250	234	188	375	285	212	316	373	276	242
280	282	266	303	267	259	364	331	263	126	296
281	321	230	251	347	177	171	306	278	293	32
417	0	389	237	381	303	256	287	246	327	0
217	154	349	249	999	321	183	367	295	247	341
233	298	160	210	336	350	285	273	369	374	187
253	289	329	210	172	259	309	295	167	153	308
170	220	272	226	337	93	243	256	305	0	247
0	300	4	251	323	323	259	123	206	321	373
159	267	351	287	281	245	245	251	331	255	176
295	174	327	266	280	373	284	326	375	242	273
186	243	414	314	220	258	177	203	236	205	401
203	186	288	359	340	297	323	282	128	275	267
255	321	153	264	259	56	248	58	320	249	226
257	255	299	326	301	319	192	296	263	155	

469

1710.6_1274EC17	322	299	4	399	387	307	303	284	633	275
341	323	284	386	428	478	287	383	444	383	348
452	240	493	280	274	449	327	377	508	469	496
508	522	455	549	748	2	689	383	367	285	373
290	342	593	359	189	408	369	268	371	305	480
339	660	664	682	303	330	660	359	800	255	462
355	796	453	471	230	460	290	472	402	395	350
390	414	301	445	365	536	205	419	479	623	724
717	677	703	228	738	123	658	609	656	710	636
707	641	683	154	694	160	678	236	310	716	718
331	655	669	742	370	437	245	513	319	513	510
429	252	279	655	605	449	262	200	375	395	588
305	331	283	347	298	148	135	322	324	301	234
336	201	425	535	455	435	438	508	469	490	439
506	588	449	588	599	514	573	520	671	586	661
488	121	321	602	558	566	297	426	308	500	432
422	381	477	471	153	331	373	499	512	131	372
383	513	192	78	293	303	671	237	94	353	218
225	423	493	219	372	295	321	476	437	207	276
291	8	266	405	342	429	329	313	388	167	538
285	726	74	233	274	4	256	247	512	376	230
475	0	509	307	407	302	364	337	546	679	22
200	225	392	484	321	999	137	435	620	817	615
204	280	215	271	413	231	384	132	622	309	614
132	614	725	466	493	300	235	442	184	118	601
346	552	592	327	167	293	757	341	726	86	627
222	539	174	602	299	451	706	250	738	398	691
551	668	215	594	339	314	85	307	299	574	612
455	247	267	625	618	702	381	577	710	341	280
232	300	667	503	533	623	312	408	581	434	594
340	386	654	601	590	490	480	632	309	467	483
563	486	171	397	584	78	518	139	585	581	554
406	455	297	331	307	346	156	386	284	315	

470

1720.9_1313EC36	159	261	110	290	274	154	269	124	158	230
191	109	303	241	175	240	253	226	219	227	206
218	192	178	231	229	229	228	190	223	239	168
226	191	132	156	195	130	207	263	206	211	282
350	269	155	193	110	363	275	213	260	311	159
191	243	229	238	264	203	227	258	181	243	239
288	196	242	243	217	255	262	250	264	165	532
130	242	275	241	186	278	196	431	220	268	243
246	236	220	272	227	221	257	197	253	204	224
187	263	261	167	240	187	261	280	382	186	213
157	202	199	183	224	233	244	191	194	225	131
252	270	204	212	166	159	153	252	263	284	169
209	276	270	212	224	280	178	106	289	243	215
192	360	275	294	283	289	289	316	273	291	241
210	211	154	237	236	230	251	235	249	252	255
275	157	135	195	243	235	235	258	247	209	254
230	3	247	141	188	215	248	276	231	200	235
240	239	223	154	148	269	82	135	180	133	21
249	211	104	8	138	222	5	90	224	188	355
65	248	137	187	230	186	279	287	58	240	138
120	195	81	156	171	0	348	381	98	156	130
197	0	199	210	186	278	151	239	171	252	149
164	152	185	0	183	137	999	182	119	200	248
156	30	166	287	1	300	251	237	156	519	160
144	256	216	8	173	164	224	183	46	263	300
188	1	268	138	319	273	248	28	125	0	293
0	202	98	110	366	48	218	69	188	194	240
208	150	297	245	57	225	191	209	214	197	189
67	0	132	221	216	214	134	193	369	214	173
178	201	255	165	1	211	142	239	241	204	179
136	198	203	332	352	262	177	193	3	107	201
162	315	116	172	208	179	8	120	196	99	169
210	97	261	274	279	255	78	247	213	166	

471

1723.7_1160EC15	307	294	196	369	358	302	330	254	364	275
300	310	330	400	333	353	346	374	267	381	365
440	232	363	322	277	396	342	378	299	453	299
293	287	365	339	432	230	444	380	392	392	290
308	361	383	350	157	383	395	249	397	362	339
337	404	387	400	379	302	383	327	448	239	319
302	435	313	326	275	378	303	312	317	290	369
333	252	389	326	313	400	205	301	371	412	442
446	404	433	322	435	170	390	360	397	487	396
484	388	384	218	403	200	391	288	381	464	463
278	384	394	419	385	287	291	380	253	410	317
302	314	266	384	352	299	230	307	336	439	373
288	277	286	296	427	284	189	406	295	288	259
264	297	355	405	380	373	361	403	383	368	354
353	375	388	376	368	377	363	319	424	362	440
386	189	280	321	356	354	240	296	98	304	306
310	193	307	311	217	269	371	355	341	199	364
334	315	158	241	270	330	374	249	202	321	202
316	326	265	204	339	334	274	345	444	251	249
273	241	304	356	394	308	439	356	288	191	357
443	426	313	165	403	111	289	289	352	356	184
273	0	350	259	391	376	345	346	299	441	59
239	200	340	319	367	435	182	999	361	443	396
170	260	287	276	269	333	296	152	505	374	407
214	372	463	360	326	292	339	363	231	151	430
238	359	405	273	314	191	446	321	399	87	351
0	276	124	354	341	297	392	249	413	414	486
373	398	364	372	247	328	225	270	313	381	435
459	224	278	377	406	438	303	397	439	363	360
233	283	460	403	352	430	296	379	442	350	356
334	287	465	428	426	400	430	428	222	365	322
345	402	179	239	355	152	316	174	373	373	334
294	330	291	319	322	318	251	324	277	283	

472

1726.7_1313EC36	332	279	1	321	346	307	323	243	604	231
311	451	385	341	455	485	312	418	437	367	350
384	163	491	314	264	404	350	272	563	364	578
567	600	422	540	661	0	576	330	381	259	342
336	363	551	319	222	389	397	242	383	307	447
327	561	552	561	336	323	553	308	618	265	614
296	621	583	624	255	306	317	591	407	293	313
346	388	270	399	362	379	180	389	455	552	565
595	596	576	313	577	127	542	492	549	617	593
609	536	533	180	558	189	555	266	304	598	595
348	540	549	597	325	381	220	546	258	556	427
421	265	208	522	510	396	207	279	398	313	414
296	243	263	263	238	136	152	310	289	283	155
259	187	369	428	384	369	353	387	367	430	347
410	468	428	510	513	399	513	418	536	482	569
402	1	338	468	485	466	203	375	147	368	371
365	343	361	372	1	195	267	359	403	0	326
374	429	141	179	271	323	593	145	161	463	247
342	424	464	282	406	291	323	537	409	139	216
399	20	394	458	147	462	251	279	415	322	523
286	642	13	236	369	2	296	241	482	321	219
396	0	396	288	264	310	346	359	575	612	0
151	134	354	525	295	620	119	361	999	635	474
200	422	309	241	410	241	329	173	485	300	545
211	488	600	449	423	289	103	396	232	118	563
330	517	501	319	209	344	583	310	543	32	472
25	487	113	508	255	389	586	250	594	325	574
454	543	277	454	303	272	137	282	332	452	423
329	251	381	518	498	662	394	508	584	309	212
204	266	538	505	440	443	266	320	481	336	676
338	326	444	508	482	397	374	462	263	472	384
399	389	179	420	442	5	447	125	486	485	440
294	382	226	203	131	293	211	249	158	227	

473

1731.5_1313EC36	315	299	11	369	359	289	381	266	695	264
285	372	302	359	415	465	307	360	390	378	423
482	223	506	289	251	439	336	360	571	448	543
551	548	459	521	847	8	749	396	390	314	348
323	331	647	360	209	354	330	226	330	316	510
355	800	793	796	347	319	788	327	942	272	481
333	980	520	488	281	420	294	498	368	399	304
382	472	258	440	369	488	209	442	497	700	806
799	726	818	319	797	107	759	690	794	819	696
819	768	800	44	820	120	806	231	285	812	812
357	794	808	893	365	473	267	526	343	530	611
493	269	309	765	723	459	271	211	377	395	615
349	340	273	345	337	137	46	348	289	283	187
298	173	456	517	469	441	469	495	441	484	444
503	653	470	685	705	480	680	577	784	681	767
508	12	326	704	653	666	232	446	300	498	463
429	432	497	527	10	338	329	528	562	15	400
390	410	127	196	273	381	715	233	178	374	65
291	468	534	214	352	354	411	398	465	272	233
294	112	252	397	344	396	314	304	344	193	546
256	808	221	258	316	3	324	246	574	337	256
421	0	450	281	370	282	371	340	680	799	65
234	174	388	425	247	817	200	443	635	999	611
350	427	326	244	445	211	380	31	648	298	676
162	570	734	505	597	288	219	401	149	179	683
295	690	685	335	196	288	824	436	804	40	699
284	648	99	688	258	463	851	236	867	400	756
660	768	176	701	373	269	121	346	250	679	630
476	242	366	706	730	777	476	578	718	313	266
203	332	708	600	651	611	312	439	643	464	589
449	388	609	634	639	521	490	677	338	516	471
578	510	219	486	625	95	617	107	656	674	680
332	476	279	335	262	299	236	348	207	335	

474

1735.8_1313EC75	359	362	192	310	288	336	347	482	556	320
294	333	355	400	369	498	304	357	320	380	409
405	270	449	331	306	472	373	324	462	401	423
462	469	434	471	613	212	580	427	376	314	356
286	340	474	382	235	393	371	336	338	328	431
340	509	525	541	307	403	522	560	578	553	421
554	592	421	429	523	742	326	434	395	573	302
573	445	310	457	374	485	272	453	463	457	507
525	489	521	301	541	219	476	563	482	600	484
600	469	481	299	495	255	484	274	294	622	620
350	490	497	529	329	423	279	477	338	468	374
407	244	203	447	439	353	315	272	384	444	466
337	357	258	277	334	268	259	326	249	268	258
340	267	503	540	528	500	530	551	517	503	534
528	492	461	535	556	453	515	466	547	503	562
438	266	314	518	534	529	246	365	193	355	378
355	341	341	319	315	299	420	367	468	317	334
401	444	224	229	329	347	560	496	236	357	171
320	475	408	325	412	362	340	401	415	254	323
354	273	326	396	300	412	433	401	414	221	465
247	594	303	275	352	135	269	309	398	374	233
424	174	445	261	385	261	355	397	518	568	42
326	282	426	427	341	615	248	396	474	611	999
294	356	266	335	374	303	596	205	524	319	434
222	525	532	371	471	558	297	434	338	192	587
354	555	491	344	278	417	528	400	500	217	519
229	439	170	461	272	477	507	252	524	342	616
523	486	287	508	561	379	286	362	303	512	498
534	482	330	486	460	534	276	484	538	416	355
157	376	487	404	540	669	381	508	457	561	479
551	456	577	402	440	581	544	530	321	509	524
492	607	336	421	538	164	529	277	554	550	522
459	506	451	471	418	464	337	479	444	338	



475

1739.1_1274EC11	164	180	93	262	270	187	332	209	363	209
	262	196	222	211	223	237	262	210	139	279
	278	170	188	199	179	226	242	152	353	252
	404	371	279	216	328	127	325	256	269	203
	202	219	346	295	60	397	340	238	208	223
	198	288	281	277	279	214	274	328	307	210
	265	326	309	279	231	330	220	291	279	203
	235	298	251	291	211	438	203	337	320	384
	333	361	347	229	347	215	349	355	358	340
	333	348	356	110	365	119	362	273	214	329
	192	320	300	303	211	268	209	398	223	395
	306	260	234	317	311	286	213	266	217	309
	225	341	243	256	249	198	108	162	367	279
	227	196	271	338	321	335	307	389	303	371
	256	293	267	297	294	259	284	274	330	341
	260	121	139	279	287	296	239	225	141	291
	197	141	280	271	157	263	340	266	292	111
	189	224	196	206	167	332	392	198	208	106
	166	209	302	154	272	235	209	309	256	154
	153	184	232	231	213	181	232	265	225	0
	167	338	32	241	246	2	244	140	293	201
	283	0	269	227	293	253	159	320	291	312
	95	176	241	215	233	204	156	170	200	350
	999	130	107	277	246	212	140	159	262	180
	60	407	304	111	302	75	220	252	206	210
	233	272	389	172	184	131	347	319	286	13
	7	329	3	334	198	281	313	77	349	109
	309	319	222	362	212	192	240	208	225	337
	149	20	199	431	375	372	340	278	358	222
	170	204	350	402	252	333	212	236	215	248
	287	221	266	353	322	333	254	277	102	247
	176	294	115	290	303	49	228	76	285	282
	255	198	260	253	333	329	204	325	308	169

476

1747.3_1313EC36	263	199	175	350	319	214	297	205	375	249
280	223	304	344	419	461	328	294	437	297	293
263	110	311	256	207	398	278	234	345	250	389
348	347	405	404	408	24	353	275	307	260	352
372	312	424	252	112	469	399	125	282	275	367
255	299	303	298	304	236	322	267	411	235	327
266	391	294	287	247	289	280	285	380	352	315
307	331	229	409	354	474	120	331	375	325	348
349	348	354	317	375	145	378	305	377	323	342
351	379	388	20	389	138	384	142	280	322	322
301	343	343	359	250	358	207	340	183	361	388
306	263	125	362	391	371	79	197	307	204	309
214	204	284	224	234	116	21	265	280	279	210
164	136	344	303	344	328	317	337	341	353	342
350	343	374	291	298	325	329	314	282	301	299
315	16	13	294	320	296	172	412	125	315	390
359	360	327	391	93	213	162	363	266	111	356
322	408	171	202	218	297	424	85	183	249	128
326	479	339	315	321	288	408	324	242	114	115
334	4	247	268	68	425	232	191	460	199	379
217	423	17	313	339	1	363	310	408	294	151
378	0	424	331	188	215	293	291	393	336	3
8	75	236	365	298	280	30	260	422	427	356
130	999	364	278	311	166	356	28	377	275	349
53	378	407	369	327	308	12	522	5	43	388
291	458	272	73	179	307	373	98	245	2	170
0	313	0	404	217	476	427	311	439	301	307
403	421	242	341	301	164	110	64	219	384	363
79	174	321	297	315	382	9	387	389	168	96
256	63	393	288	349	361	193	353	340	362	451
364	357	276	396	382	313	252	268	135	429	349
356	263	2	351	262	0	393	1	320	363	330
310	362	137	74	16	199	170	140	182	168	

477

1755.7_1313EC75	204	186	130	231	274	194	249	234	269	177
331	235	384	256	328	338	255	231	311	268	261
267	144	245	333	432	304	405	216	311	291	275
313	328	312	381	304	118	264	209	280	244	273
229	386	385	235	139	338	269	194	308	332	232
217	227	249	230	309	210	220	343	319	337	253
317	295	205	252	338	270	374	252	262	373	265
371	335	298	234	258	300	209	288	319	293	202
229	257	217	235	245	190	268	290	276	227	276
199	247	326	6	296	150	306	322	328	198	196
190	327	326	314	271	223	102	298	162	302	252
203	190	116	255	258	242	218	322	179	301	281
213	207	221	160	182	212	6	222	264	295	195
221	213	341	327	339	356	359	380	355	373	336
296	285	241	263	297	217	292	247	243	299	241
276	5	70	260	294	304	167	288	170	274	281
246	214	291	267	6	137	287	284	240	5	222
271	316	41	281	182	249	288	207	198	227	280
406	301	287	301	319	265	249	267	252	220	148
251	242	209	303	150	312	234	181	361	191	356
134	264	21	226	285	158	226	303	383	268	159
284	0	254	247	217	227	231	259	387	268	0
173	167	199	292	160	215	166	287	309	326	266
107	364	999	139	247	326	406	227	302	258	251
257	321	247	267	284	412	256	331	252	136	273
235	359	254	136	291	193	220	176	259	102	176
241	257	0	323	297	381	334	365	325	278	287
344	269	317	278	215	199	234	137	351	325	285
218	217	381	269	283	286	195	426	308	234	176
211	143	296	342	317	221	277	329	375	310	325
334	293	223	344	275	328	296	277	107	343	241
287	307	236	285	228	69	301	154	268	354	251
190	263	257	261	213	301	309	260	242	163	

478

1758.1_1313EC75	341	348	398	310	303	317	284	209	276	209
324	286	284	296	272	326	268	284	316	327	243
296	354	280	305	316	361	312	287	326	289	281
312	321	277	239	236	397	359	422	261	248	289
264	300	279	214	156	344	309	203	314	308	296
256	250	253	237	232	312	244	269	208	230	254
257	242	278	253	249	317	327	255	357	300	356
282	293	336	288	278	378	208	315	334	307	254
254	295	249	242	273	287	259	265	279	280	310
296	238	244	432	299	197	293	292	349	306	323
227	230	221	238	269	246	298	303	256	305	314
236	284	256	258	255	240	156	244	229	347	244
266	312	309	243	291	332	411	211	385	287	313
220	374	257	308	275	303	263	318	287	329	252
285	259	252	269	262	270	262	258	261	260	279
270	404	213	253	256	252	256	212	155	218	280
219	60	250	174	429	235	319	310	301	425	333
320	336	206	231	310	284	234	135	187	337	226
215	226	280	254	296	251	201	267	301	235	330
254	190	313	330	265	338	374	373	282	146	237
262	256	165	175	269	79	244	276	295	221	120
252	0	270	284	338	248	262	264	243	267	54
284	191	337	228	210	271	287	276	241	244	335
277	278	139	999	287	365	307	134	210	329	206
170	341	278	78	188	228	291	197	216	255	378
233	259	282	218	318	182	229	124	237	48	280
0	257	132	209	340	212	207	70	221	282	289
215	235	284	251	305	332	281	261	240	263	240
240	5	190	390	238	302	168	264	369	324	372
167	264	364	227	254	259	180	196	253	238	242
228	193	328	287	352	264	349	251	139	367	282
261	263	28	248	274	110	205	140	218	231	199
318	205	386	386	319	331	189	310	251	283	

479

1761.3_1313EC75	253	233	145	306	317	216	222	251	442	314
446	293	226	332	344	359	272	258	307	325	247
300	127	319	255	199	264	335	247	393	281	389
413	397	421	343	478	0	456	241	371	205	397
311	288	386	221	145	315	270	227	249	227	337
270	395	416	423	213	414	419	314	407	309	344
317	412	386	360	303	308	266	365	360	236	309
304	298	331	311	261	359	181	390	325	399	460
449	379	439	244	440	129	421	425	416	423	397
429	406	382	115	388	132	381	253	259	431	435
224	434	451	461	290	341	166	400	201	411	290
328	237	197	384	353	331	157	239	296	285	349
210	231	281	258	195	181	177	215	244	223	133
208	187	343	413	345	350	324	372	357	379	270
334	354	312	417	425	335	414	333	423	380	424
311	116	165	431	397	393	173	306	174	357	309
337	235	331	311	48	163	281	311	343	2	340
297	383	157	10	205	222	463	256	79	337	304
282	262	291	159	326	294	276	313	253	192	204
257	107	235	355	205	332	271	314	392	312	374
222	464	1	201	344	0	302	248	369	220	177
474	128	371	301	356	201	288	323	393	406	89
174	46	431	432	336	413	1	269	410	445	374
246	311	247	287	999	229	257	31	368	216	389
115	708	442	256	364	281	202	297	219	120	470
188	428	403	181	202	233	453	273	424	42	390
249	411	129	386	211	259	461	158	489	314	411
377	400	274	386	311	226	199	177	245	361	316
262	93	239	419	422	448	192	304	414	249	179
167	186	368	407	387	391	216	256	357	311	470
278	301	394	362	358	358	351	378	278	315	375
324	373	262	374	372	34	362	140	393	365	372
288	305	229	213	183	277	239	278	258	155	

480

1763.9_1313EC75	336	366	222	346	361	338	391	176	247	251
395	345	564	433	254	288	373	253	247	364	330
359	234	260	574	282	287	528	356	298	382	266
312	279	205	227	224	226	272	480	360	347	295
279	616	255	252	207	343	343	296	355	642	246
309	229	243	236	335	328	239	308	199	256	248
277	235	240	251	296	272	635	231	213	189	337
191	208	697	211	258	292	217	302	254	307	236
220	273	247	303	237	231	206	230	207	227	272
236	196	167	199	187	224	185	603	577	244	255
217	188	188	185	320	234	321	265	244	263	193
202	271	199	198	184	203	239	652	296	384	192
245	330	238	205	306	618	216	304	339	300	206
258	580	194	252	229	233	207	254	283	275	210
181	209	252	248	235	232	248	178	242	269	265
261	206	193	183	250	242	218	194	65	220	211
197	135	204	185	183	177	302	239	214	176	313
335	328	119	633	314	391	255	141	231	346	267
575	230	267	191	264	305	145	289	356	241	312
270	598	332	336	338	240	474	513	224	201	244
297	248	210	213	345	305	244	511	285	298	231
166	0	190	466	514	352	271	462	224	267	152
216	103	365	252	350	231	300	333	241	211	303
212	166	326	365	229	999	247	447	202	341	205
545	259	266	184	174	212	665	188	225	262	304
207	160	310	204	672	157	223	194	206	59	284
1	199	171	156	556	161	169	219	191	309	299
189	223	780	273	258	251	475	246	647	232	203
209	13	614	275	226	386	495	482	451	270	296
204	241	422	266	220	199	164	148	197	191	260
152	203	267	347	307	288	306	214	122	224	187
229	277	142	270	210	187	240	52	252	242	186
249	183	291	269	240	262	166	274	298	209	

481

1769.9_1313EC75	287	262	21	320	336	256	322	666	461	324
309	252	313	306	347	421	299	301	319	313	268
287	245	336	238	245	373	330	277	373	334	339
366	365	330	350	404	23	354	306	335	272	391
292	334	326	247	126	372	352	211	349	288	321
305	348	363	361	310	284	363	717	351	662	343
678	377	358	349	677	717	329	368	369	977	307
738	344	267	414	325	455	173	400	329	359	374
380	400	365	277	379	110	378	421	361	369	385
370	361	360	164	358	258	364	204	249	386	387
318	331	331	348	269	382	211	363	243	366	324
365	258	225	341	334	348	221	304	328	296	345
216	221	246	249	216	145	87	263	284	286	175
240	153	617	681	642	618	638	676	643	615	694
603	344	377	345	369	380	329	319	350	366	361
355	16	159	318	347	340	293	320	136	319	311
384	316	323	316	142	280	269	437	339	151	376
281	364	201	151	246	322	452	676	23	306	7
301	429	323	268	336	365	249	343	312	232	179
285	2	291	329	257	354	248	285	406	190	366
293	419	86	249	314	2	298	309	310	273	139
356	182	351	289	224	215	298	364	380	402	23
148	344	267	270	285	384	251	296	329	380	596
140	356	406	307	257	247	999	0	385	265	261
144	401	452	256	314	785	196	399	181	5	419
257	383	339	253	215	285	355	300	313	42	305
5	307	131	326	223	407	347	190	364	306	342
371	361	209	348	559	215	92	203	268	376	396
577	572	221	332	329	359	147	393	396	231	112
201	252	335	335	352	691	425	640	402	680	365
599	571	342	365	375	692	453	326	135	335	668
331	658	530	304	342	91	326	88	338	338	337
507	519	298	304	302	306	194	318	294	210	

482

1770.3_1274EC17	87	225	41	222	325	165	191	16	164	191
244	0	383	205	151	168	173	191	69	327	239
241	79	120	344	254	98	302	225	242	258	68
214	97	82	151	86	43	119	275	238	180	247
195	425	74	228	0	342	270	174	290	492	129
131	179	167	179	275	217	175	293	109	220	204
300	113	150	214	228	255	414	185	176	112	256
97	111	337	141	163	272	148	278	298	299	175
124	159	171	78	144	55	106	124	116	182	171
215	109	112	126	137	171	141	444	399	189	203
108	64	68	71	178	154	134	203	165	217	94
201	184	178	165	149	84	102	478	191	294	197
202	189	205	145	185	423	138	171	284	243	187
198	389	213	273	264	284	253	284	263	317	240
239	151	179	198	177	183	216	164	230	232	250
174	97	161	245	196	170	210	205	267	135	273
1	0	144	258	122	180	240	171	211	149	222
121	149	156	476	91	191	164	0	161	1	99
356	146	116	5	84	226	6	163	128	0	160
72	411	80	46	177	59	309	287	3	236	161
231	118	106	174	241	8	209	333	58	65	1
90	0	97	9	222	272	11	333	63	206	126
179	0	159	177	273	132	237	152	173	31	205
159	28	227	134	31	447	0	999	2	218	1
501	230	127	169	1	0	373	119	205	149	181
160	0	185	132	446	180	118	116	129	33	159
0	192	140	45	431	115	24	175	37	173	213
0	49	450	161	163	164	327	112	447	28	70
63	0	438	213	123	275	464	286	331	191	165
86	105	327	181	1	123	208	124	74	174	13
1	226	147	306	226	201	89	159	117	99	175
141	277	73	119	220	152	74	102	142	74	108
202	67	173	211	169	158	2	186	173	51	



483

1771.1_1274EC11	234	175	77	357	308	225	305	258	486	308
277	310	291	384	403	394	328	408	399	330	326
393	217	423	250	198	347	279	374	342	389	368
340	334	394	463	636	141	608	347	369	253	282
278	338	489	366	155	349	288	193	279	287	396
359	574	578	572	280	290	576	281	685	244	372
279	612	388	378	221	358	245	367	309	383	286
419	327	229	385	272	411	191	322	456	572	646
640	615	608	277	694	143	530	510	532	691	609
691	510	494	69	518	200	508	178	230	628	632
273	551	563	660	397	403	213	370	267	377	437
404	225	275	526	491	358	173	211	290	346	542
278	266	241	323	265	105	82	357	270	255	238
252	171	412	444	416	400	413	432	392	412	439
486	558	407	567	565	439	524	530	584	535	593
458	126	322	554	486	499	244	353	141	404	356
326	350	358	372	76	251	323	367	521	102	375
291	349	94	191	212	305	482	122	241	311	215
364	397	317	205	391	296	379	403	449	255	156
286	137	233	322	278	409	274	308	367	189	456
156	623	75	229	389	32	255	221	476	374	150
444	0	446	324	322	207	404	363	477	593	1
118	149	331	358	369	622	156	505	485	648	524
262	377	302	210	368	202	385	2	999	297	534
137	470	608	587	515	285	248	408	146	173	615
318	595	440	316	153	301	616	369	609	167	437
22	480	158	470	198	448	573	250	581	465	646
542	533	183	471	349	262	128	309	198	483	593
471	331	258	493	481	556	259	489	587	288	245
243	302	557	418	466	560	255	430	677	395	478
364	379	698	490	485	440	384	636	407	496	407
562	456	203	352	572	165	441	58	522	495	535
326	445	280	270	295	288	206	289	200	285	

484

1784.4_1313EC36	326	295	208	416	376	255	343	198	303	308
309	291	305	417	353	315	358	407	303	380	381
388	253	318	339	294	313	321	322	313	391	291
317	292	310	355	276	202	323	387	303	333	346
605	349	340	286	172	453	476	244	302	352	264
281	288	282	288	346	329	278	289	269	248	289
297	275	279	289	276	314	311	296	356	231	974
205	270	349	345	275	356	209	396	314	307	277
273	293	266	369	310	240	296	303	293	333	267
345	293	285	235	311	198	304	264	524	331	334
285	269	267	263	305	285	297	295	268	292	260
296	307	162	279	270	257	172	258	264	354	271
276	291	322	238	394	326	237	355	348	299	232
235	394	263	288	287	277	259	317	277	343	291
302	311	322	323	323	334	335	309	326	331	318
344	224	249	293	322	315	223	250	226	256	264
222	193	241	203	242	197	312	284	303	234	396
359	384	178	169	290	343	319	171	265	299	187
263	280	282	212	442	333	297	342	366	206	352
304	298	293	369	320	273	424	360	287	466	334
360	292	235	365	308	177	609	400	252	279	178
244	0	243	238	370	450	292	346	289	296	141
270	84	349	249	374	309	519	374	300	298	319
180	275	258	329	216	341	265	218	297	999	224
172	320	343	158	243	249	260	269	208	309	441
226	212	314	250	406	188	287	168	238	80	320
5	246	156	231	488	303	267	240	280	299	366
252	281	334	315	218	309	263	285	272	323	258
281	33	242	329	304	305	207	311	358	321	306
304	281	329	293	242	301	193	299	250	256	289
289	226	318	385	419	309	372	344	218	272	285
282	297	126	250	324	201	170	41	289	271	283
262	235	331	382	342	331	200	336	301	234	

485

1784.9_1313EC75	265	271	105	313	318	261	296	232	515	291
296	283	339	353	466	365	291	332	415	308	283
385	163	379	265	242	378	329	272	465	414	488
478	467	474	491	655	0	616	357	339	275	289
270	342	759	266	209	358	255	168	258	275	721
278	651	647	659	248	322	646	307	685	221	416
256	626	415	422	195	288	260	407	404	267	202
358	334	223	388	322	417	115	386	436	578	705
701	634	661	265	677	106	506	515	509	730	579
732	498	519	0	535	135	528	242	241	711	715
323	577	573	621	294	469	146	440	249	453	634
579	195	243	790	727	576	184	273	332	348	517
225	287	257	283	228	147	63	261	226	255	123
245	144	385	446	389	347	388	444	394	403	421
382	511	434	528	526	373	516	488	609	515	597
402	0	202	533	495	499	197	400	142	417	405
392	272	398	416	0	232	257	388	463	0	342
391	378	9	239	261	296	557	195	82	334	35
280	403	698	198	331	351	266	372	351	529	193
256	6	244	302	313	383	315	248	444	278	482
154	697	145	279	329	2	285	264	744	299	173
431	0	423	303	243	242	301	366	510	641	0
252	145	349	497	187	614	160	407	545	676	434
307	349	251	206	389	205	261	1	534	224	999
70	496	577	447	405	215	146	388	45	1	513
306	522	518	185	209	319	698	309	674	38	545
5	509	3	512	186	390	598	147	602	335	627
495	749	195	468	309	143	133	195	298	442	564
369	126	422	532	524	594	354	467	582	193	185
230	195	574	531	505	525	276	396	590	448	591
379	316	511	541	523	462	384	533	358	529	392
483	394	234	428	533	5	450	0	500	505	473
278	414	172	225	217	214	183	255	142	250	

486

1794.4_1274EC17	189	161	165	191	240	224	194	47	145	131
221	154	535	218	114	155	197	149	131	243	256
253	154	156	443	180	150	459	265	217	271	188
230	208	130	155	144	204	127	291	226	234	143
151	525	159	142	194	185	242	192	233	613	149
234	225	198	216	245	170	218	249	162	190	211
243	165	217	203	207	144	640	195	115	140	209
133	146	393	146	150	156	155	243	236	187	172
158	158	184	127	171	124	184	140	184	166	150
174	186	187	148	170	114	171	670	463	179	177
168	147	147	141	210	196	216	214	155	207	97
176	169	149	165	165	126	182	665	228	263	144
182	256	123	144	181	477	154	200	261	210	114
179	471	160	230	197	224	184	222	256	190	207
162	142	172	196	155	231	205	159	180	216	179
207	106	130	199	212	172	210	239	187	174	270
24	4	153	230	95	96	211	139	189	129	186
200	55	192	755	220	194	161	54	124	202	4
658	127	142	89	40	176	109	170	244	5	251
281	574	257	255	269	140	288	345	49	4	177
171	126	180	123	223	61	173	399	160	207	208
163	0	154	209	210	221	194	215	122	220	1
187	225	210	250	253	132	144	214	211	162	222
60	53	257	170	115	545	144	501	137	172	70
999	159	198	3	147	122	422	74	140	2	182
95	101	281	161	585	0	196	120	153	2	267
1	220	87	202	448	51	138	0	145	189	198
141	130	603	202	43	178	342	167	677	188	84
232	6	654	183	200	259	631	433	367	164	163
117	124	312	195	167	166	130	179	106	182	155
80	213	180	201	164	238	154	136	49	100	147
129	224	15	158	158	124	202	78	214	186	120
134	126	180	166	101	142	4	162	171	205	

487

1796.4_1313EC75	326	319	210	346	336	303	346	301	582	341
363	315	292	387	434	435	346	344	410	396	320
359	273	438	301	323	445	337	300	506	375	503
513	498	446	428	628	203	611	401	399	260	384
361	319	467	266	201	457	346	305	286	282	397
329	550	564	569	280	433	565	369	550	384	427
364	539	465	440	373	422	309	442	392	374	357
354	427	296	380	361	434	222	396	401	531	560
565	549	532	304	552	163	510	502	492	531	550
523	491	486	244	505	223	488	266	318	538	540
317	495	493	532	340	396	187	499	287	510	423
390	255	240	475	423	336	230	218	351	355	429
296	324	309	266	272	313	222	307	309	293	248
268	254	346	456	366	363	341	422	386	465	332
368	414	335	466	476	373	453	399	538	430	512
367	205	290	491	442	444	241	390	283	413	403
421	415	429	376	249	330	468	406	415	242	362
388	411	271	160	285	346	608	264	220	363	214
260	384	404	307	378	301	300	474	379	221	310
311	146	320	409	282	443	363	356	400	172	449
250	638	246	264	361	28	341	321	402	294	220
502	179	422	335	352	295	352	377	561	539	134
367	155	451	439	289	614	256	372	488	570	525
407	378	321	341	708	259	401	230	470	320	496
159	999	522	358	455	319	248	398	284	179	595
331	534	484	295	264	258	605	324	560	196	490
318	423	162	452	281	373	538	202	567	379	550
486	518	252	483	411	409	257	316	266	464	439
434	282	295	494	492	529	254	450	563	425	374
217	309	517	495	482	517	218	321	449	365	605
322	318	511	489	509	411	535	522	289	466	444
449	440	249	407	469	143	467	311	484	464	454
363	432	437	465	413	472	379	471	405	362	

488

1802.0_1313EC75	329	318	30	362	311	322	322	262	619	297
317	388	338	437	372	522	257	369	427	348	291
471	259	541	315	306	414	368	356	549	452	559
539	543	374	486	671	2	635	372	301	321	380
271	331	552	298	256	285	380	193	322	289	532
326	584	579	569	307	400	566	333	706	223	418
290	700	477	420	247	357	301	440	419	434	292
322	381	316	459	313	493	136	343	489	528	552
578	527	591	262	571	115	605	600	598	668	538
668	573	580	23	604	82	610	241	258	662	653
287	643	646	692	342	376	248	465	285	476	548
404	285	226	618	552	405	213	229	255	408	530
294	328	318	290	408	220	34	369	283	266	153
269	239	392	467	374	365	377	444	417	469	405
390	548	379	565	584	437	570	516	590	564	615
436	10	319	587	539	536	291	336	247	375	346
374	400	340	331	17	322	315	360	519	31	370
431	445	101	254	323	322	617	222	251	412	193
310	480	477	247	424	345	269	475	530	335	285
347	133	285	433	348	419	386	317	422	159	492
201	723	161	276	328	73	278	273	498	296	204
531	0	494	300	377	304	346	314	557	595	0
172	141	449	560	329	725	216	463	600	734	532
304	407	247	278	442	266	452	127	608	343	577
198	522	999	669	554	302	262	476	187	127	660
272	634	539	333	227	211	615	314	595	74	574
343	515	120	587	257	444	662	185	689	408	663
570	630	215	560	316	299	128	326	299	536	558
486	301	343	596	572	649	367	798	616	308	338
183	327	578	458	528	490	271	399	533	451	616
436	361	625	519	466	491	527	614	398	534	514
540	426	271	374	586	167	516	7	558	576	548
319	430	352	373	359	358	181	378	283	429	

489

1806.2_1313EC75	257	149	0	165	223	210	248	202	327	104
231	69	242	268	278	286	254	296	241	269	238
243	153	231	150	185	367	239	234	266	247	340
298	306	399	435	493	0	411	256	266	211	184
263	299	464	261	5	311	241	199	257	244	313
228	417	424	447	264	137	418	254	514	171	304
216	503	266	306	139	225	163	304	250	243	203
320	305	104	315	257	377	163	271	409	442	457
465	492	466	308	447	164	440	357	452	443	501
443	449	429	0	441	160	423	247	185	421	420
217	423	427	430	294	267	149	366	213	379	357
272	218	193	384	351	314	172	224	280	232	344
172	171	162	221	107	70	0	249	211	245	8
189	89	354	354	325	324	309	352	345	363	302
377	442	352	362	358	334	396	378	397	387	417
317	0	12	361	390	378	192	311	14	304	306
257	254	325	317	0	157	300	297	364	0	264
86	302	1	241	168	248	329	238	168	97	11
306	332	267	221	248	268	182	250	207	135	2
140	1	155	175	166	298	94	160	354	6	383
201	431	61	263	250	3	258	145	386	263	7
279	0	347	354	192	154	243	316	405	429	0
49	149	200	258	210	466	8	360	449	505	371
111	369	267	78	256	184	256	169	587	158	447
3	358	669	999	342	47	155	345	91	169	333
177	441	352	181	74	309	490	341	464	119	276
0	311	2	371	141	400	393	214	454	285	519
436	428	154	435	131	176	47	162	176	418	437
338	269	256	368	378	413	41	545	422	207	80
206	202	423	324	377	424	169	388	475	333	293
300	321	442	384	388	362	206	407	266	406	346
353	331	198	240	348	6	371	0	353	395	355
214	332	109	127	105	163	315	203	218	61	

490

1806.4_1274EC17	221	298	60	287	299	203	243	246	486	217
284	318	240	245	323	334	266	280	310	356	490
368	147	446	192	240	388	275	244	360	331	365
368	377	353	440	633	86	591	261	316	239	271
236	286	447	285	131	318	281	236	228	296	467
353	480	472	474	227	301	468	273	565	234	394
254	555	414	413	231	345	258	415	267	292	246
286	646	217	413	280	437	230	306	521	478	494
483	466	503	276	486	178	527	716	539	614	452
615	529	532	139	534	238	528	243	283	633	631
326	534	547	591	297	451	235	399	296	402	436
427	244	334	512	531	402	226	247	321	350	565
276	296	259	379	273	110	122	230	315	296	205
289	141	395	379	408	397	390	431	382	407	418
459	471	313	663	677	391	607	604	611	614	625
368	169	281	657	626	614	245	413	176	379	418
412	441	363	404	231	339	286	453	518	230	314
314	324	138	188	199	243	519	245	84	266	149
220	315	375	204	282	307	576	293	331	279	170
247	117	215	275	235	339	251	217	314	330	435
249	630	1	229	285	1	251	202	401	281	228
440	1	360	253	339	247	357	297	632	497	0
102	252	311	313	172	493	173	326	423	597	471
302	327	284	188	364	174	314	1	515	243	405
147	455	554	342	999	218	171	335	160	3	595
252	908	478	259	163	240	505	618	459	127	425
723	428	1	462	188	378	586	206	589	353	583
922	559	177	694	258	272	183	278	243	643	587
351	59	309	488	472	513	286	465	433	313	259
194	280	420	421	777	443	323	389	430	382	413
563	415	503	436	425	400	337	580	283	362	453
590	552	105	491	633	117	652	105	636	617	832
266	415	249	249	265	229	241	307	216	251	



491

1813.0_1313EC75	300	227	9	243	322	263	303	597	392	287
322	249	305	320	359	369	291	308	450	366	333
315	217	269	271	280	384	329	292	312	271	296
315	311	301	395	353	0	266	275	341	273	348
296	283	284	305	127	322	279	194	272	271	316
311	251	269	263	334	256	269	669	262	731	291
654	311	247	295	656	630	275	259	368	778	268
906	356	236	351	285	413	174	317	308	295	278
285	283	293	242	278	71	283	359	285	295	275
297	289	291	2	289	221	289	182	243	276	272
249	255	255	259	317	254	169	332	223	337	273
250	253	157	273	260	269	203	293	318	323	258
200	189	241	212	239	165	4	236	299	254	167
225	184	655	654	663	666	667	666	647	614	720
581	220	223	221	219	309	217	201	251	232	248
274	0	58	226	237	226	243	356	144	309	318
359	261	336	360	79	187	213	328	229	0	299
345	488	152	67	264	303	383	579	24	301	82
278	348	292	156	396	372	305	333	360	191	164
306	154	284	291	143	414	217	262	336	226	390
209	371	130	222	342	0	301	260	329	300	166
312	218	271	322	196	198	307	398	295	285	164
156	292	251	350	259	300	164	292	289	288	558
75	308	412	228	281	212	785	0	285	249	215
122	319	302	47	218	999	107	383	104	0	301
280	303	285	181	203	322	285	269	242	10	217
0	183	126	263	236	405	269	227	289	324	267
241	347	157	238	572	181	108	146	271	271	308
550	591	199	257	235	326	12	303	302	203	89
178	234	292	306	304	636	497	676	318	682	306
590	566	239	292	316	660	358	200	173	271	601
233	599	545	252	202	144	230	11	268	261	243
480	486	237	233	229	292	170	260	213	208	

492

1819.8_1313EC75	284	308	195	391	357	283	366	125	217	311
577	262	407	412	209	216	330	205	107	353	355
336	234	202	453	246	219	400	349	241	350	180
257	176	188	221	222	185	271	389	324	323	295
266	527	205	251	166	274	306	221	303	500	209
310	247	248	253	299	307	253	310	228	285	257
267	195	240	245	314	241	471	218	164	174	279
202	172	903	212	162	266	193	266	230	271	247
243	217	229	264	245	215	198	234	198	237	255
242	198	162	188	185	216	183	448	493	263	255
167	174	173	192	326	216	234	258	238	264	169
206	243	191	185	185	138	256	453	251	387	188
257	301	255	181	300	624	195	285	301	276	163
262	572	196	236	228	269	232	259	296	299	242
177	189	190	221	220	241	231	193	233	250	248
239	188	185	204	249	248	191	130	21	190	195
59	93	180	149	206	195	281	157	229	148	349
283	253	159	498	275	366	261	155	270	276	607
406	102	241	202	195	272	212	250	330	222	278
219	468	290	312	362	138	484	573	166	145	224
298	226	226	181	332	271	234	379	242	318	171
114	0	140	462	614	312	281	440	170	244	143
228	110	339	172	309	235	224	339	103	219	297
220	12	256	291	202	665	196	373	248	260	146
422	248	262	155	171	107	999	174	264	303	330
202	149	277	200	606	199	236	231	186	134	283
14	184	193	132	498	96	150	144	159	300	320
186	148	643	267	174	238	508	242	521	228	131
250	2	436	252	191	315	397	344	329	228	267
186	248	384	201	204	174	180	148	184	198	220
170	126	262	270	242	277	268	234	79	77	218
208	246	138	214	231	232	222	55	264	239	212
225	174	287	288	264	280	147	288	284	204	

493

1822.5_1313EC75	284	222	15	297	341	253	305	274	449	245
301	261	271	332	485	504	357	302	425	292	299
303	192	380	258	292	418	304	251	406	293	379
395	384	442	469	426	79	366	263	341	288	353
302	332	403	284	146	345	373	197	253	283	394
252	285	352	350	354	328	343	319	402	302	393
327	422	403	394	333	327	265	381	502	366	284
387	307	216	773	290	955	198	282	383	356	385
391	429	408	351	425	107	409	394	404	421	350
439	402	397	52	400	189	406	196	273	402	420
266	319	331	359	275	314	144	397	262	397	331
283	233	261	418	373	303	251	218	276	316	406
314	267	257	256	260	123	49	249	257	258	237
267	133	288	306	301	310	274	371	315	418	336
298	417	282	340	378	345	353	346	334	338	339
307	108	268	385	360	373	219	346	155	325	345
271	336	321	320	56	166	255	285	371	51	368
363	428	27	163	255	305	436	223	164	306	68
311	482	334	261	378	353	330	396	305	350	173
329	1	283	337	161	472	287	254	470	173	456
236	490	137	274	339	0	317	293	394	337	164
460	0	508	264	231	232	288	268	411	394	0
125	168	322	432	295	442	183	363	396	401	434
252	522	331	197	297	188	399	119	408	269	388
74	398	476	345	335	383	174	999	120	72	389
289	386	328	274	152	323	388	228	307	225	281
1	285	165	382	235	501	352	203	367	309	376
363	451	199	345	301	202	112	257	224	369	474
315	197	315	287	315	386	107	460	376	221	178
209	258	342	357	336	358	225	329	325	349	379
355	299	342	400	369	335	372	416	216	387	408
332	289	168	343	392	209	359	58	382	418	305
238	356	373	318	355	316	217	317	257	348	

494

1824.3_1191EC08	191	313	157	194	256	191	259	199	203	188
287	123	207	203	208	248	207	195	118	339	190
232	180	236	138	245	197	232	254	247	221	139
242	203	186	254	182	197	198	225	231	205	225
245	214	101	208	146	393	248	306	301	232	180
251	264	235	196	238	218	250	346	167	244	223
339	185	240	207	240	351	283	181	248	216	283
205	261	284	195	270	382	361	182	272	347	221
216	229	236	107	222	376	268	203	269	251	225
265	256	264	205	270	229	274	313	286	293	286
212	177	161	177	326	205	167	264	290	258	194
216	235	248	224	211	182	235	234	337	370	228
309	291	294	268	255	252	212	169	313	254	265
296	208	295	328	319	326	292	361	361	397	292
274	192	206	269	276	338	267	230	294	314	314
357	230	49	199	249	248	257	264	86	269	294
170	161	269	251	213	166	346	242	272	224	206
113	239	325	29	142	259	168	205	206	151	112
117	143	136	239	81	202	136	137	244	120	182
123	216	205	154	153	187	253	178	30	4	209
206	232	98	25	168	57	175	190	137	151	139
250	184	131	134	224	194	233	228	162	250	121
184	166	223	7	167	184	46	231	232	149	338
206	5	252	216	219	225	181	205	146	208	45
140	284	187	91	160	104	264	120	999	115	209
224	166	220	137	225	273	186	208	164	209	222
163	228	155	127	226	152	161	184	166	255	232
156	183	262	240	172	258	297	188	260	143	211
74	208	224	289	225	180	139	126	176	239	273
130	200	233	279	119	207	222	167	198	261	3
145	179	206	320	267	249	224	205	43	167	224
189	317	122	216	270	77	122	123	225	153	178
292	134	280	266	197	218	181	300	254	149	

495

1827.9_1313EC75	119	233	174	88	175	54	176	98	41	145
372	130	75	157	199	146	172	212	267	177	111
96	198	0	141	257	49	85	96	68	151	3
101	95	204	86	46	175	123	140	171	163	193
258	149	125	78	0	239	207	72	217	160	89
99	214	161	162	163	185	151	201	192	149	245
152	206	191	248	166	227	172	208	222	179	320
127	172	315	203	134	239	155	349	233	234	166
141	199	174	106	171	246	204	196	202	179	208
184	209	201	192	215	72	204	138	278	211	200
0	216	219	214	96	218	218	229	183	228	153
207	211	118	261	161	138	0	88	112	229	231
168	152	283	180	207	205	207	12	259	154	257
155	257	312	261	299	304	291	291	189	227	234
239	225	124	211	200	252	209	197	246	205	227
228	224	5	190	200	195	227	243	200	170	224
229	1	186	132	221	240	199	184	174	206	116
95	212	168	9	57	176	0	96	123	6	344
4	114	74	199	146	88	0	1	134	2	191
2	142	135	118	171	140	269	244	12	111	62
82	148	138	105	60	2	236	159	2	12	0
184	0	193	310	303	213	5	187	83	165	26
150	139	181	1	153	118	263	151	118	179	192
210	43	136	255	120	262	5	149	173	309	1
2	179	127	169	3	0	303	72	115	999	166
75	0	255	10	198	74	143	3	114	1	250
0	270	0	331	234	43	217	112	141	5	196
2	86	204	157	148	183	172	143	183	22	223
6	5	144	299	285	217	18	127	168	172	144
87	130	258	134	0	214	103	274	126	160	21
219	163	195	163	212	225	66	170	3	229	214
83	175	5	86	174	2	3	0	126	8	171
206	143	240	221	196	190	6	200	183	35	

496

1835.3_1313EC75	324	341	201	439	402	335	376	323	597	339
347	400	351	434	431	445	367	398	364	460	448
533	267	526	367	258	473	379	405	496	553	454
516	465	491	533	667	234	630	477	491	350	454
365	376	526	415	193	504	491	331	380	342	511
432	585	584	590	408	482	578	369	648	340	522
375	643	533	539	318	438	325	545	410	404	471
417	459	345	460	323	502	231	515	484	592	614
625	578	626	308	636	188	591	605	593	668	571
671	586	572	225	598	207	583	293	425	655	658
320	564	572	631	413	446	292	476	327	476	472
448	362	354	547	518	433	240	286	406	472	561
334	377	300	391	392	281	217	404	379	378	264
303	272	433	510	462	450	456	522	467	537	460
501	538	448	624	627	467	584	545	631	569	632
474	214	326	573	571	583	244	424	152	398	439
380	357	392	429	224	299	383	477	468	261	432
437	469	197	211	305	376	634	285	240	416	200
282	412	438	243	376	323	428	476	535	351	340
313	194	307	408	428	403	343	438	460	136	542
306	670	123	326	432	48	354	345	463	431	227
473	0	465	305	456	423	449	325	580	646	88
279	136	540	474	308	601	300	430	563	683	587
340	388	273	378	470	304	419	181	615	441	513
182	595	660	333	595	301	330	389	209	166	999
242	658	580	325	280	233	636	463	628	114	562
396	507	129	505	386	466	631	222	645	420	647
625	583	285	626	311	368	249	347	337	609	625
461	240	336	605	568	600	330	509	579	395	404
344	338	625	538	600	586	343	431	571	457	552
457	461	566	587	573	540	496	611	306	457	512
567	513	249	463	590	129	545	165	609	580	587
352	462	354	406	357	419	203	421	332	349	

497

1842.1_1313EC75	179	267	239	179	260	193	218	221	381	221
271	235	201	255	333	366	233	237	330	297	197
226	173	278	184	314	314	264	184	361	207	343
368	377	281	328	307	223	364	166	278	202	214
206	209	292	139	146	359	254	163	265	200	272
133	175	256	221	184	248	223	304	247	228	237
270	280	250	240	227	268	211	257	305	241	186
216	287	223	284	198	327	204	213	302	285	227
231	271	216	179	233	136	305	295	292	303	201
290	231	243	240	256	171	229	169	202	317	302
219	293	293	298	202	233	103	379	214	377	287
234	228	170	260	266	276	185	168	182	257	283
179	239	256	198	165	172	250	119	255	214	226
221	176	258	275	255	286	271	301	294	307	278
307	329	234	332	318	303	315	267	362	342	354
284	270	206	311	308	312	207	246	214	258	236
263	240	237	209	305	150	321	240	336	290	237
289	365	237	122	182	218	390	213	174	274	12
246	339	274	324	273	261	262	358	303	172	195
306	155	217	265	144	394	340	213	320	144	333
195	273	29	228	325	0	224	184	256	216	141
300	172	281	275	255	179	157	244	289	285	87
224	103	206	238	170	346	188	238	330	295	354
233	291	235	233	188	207	257	160	318	226	306
95	331	272	177	252	280	202	289	224	75	242
999	295	258	271	175	485	226	189	156	118	242
3	328	172	326	154	301	308	231	305	253	377
233	274	231	264	363	304	192	274	162	252	202
158	19	193	334	255	331	38	254	303	348	284
196	275	273	288	191	199	250	203	229	183	318
234	254	365	316	343	176	375	315	107	383	220
279	307	69	353	299	161	214	306	302	324	261
409	282	368	334	332	317	323	336	292	184	

498

1843.5_1313EC36	298	322	0	360	375	224	291	320	581	296
319	325	316	302	403	397	324	341	393	374	517
365	141	396	208	228	443	316	231	466	336	456
463	459	409	491	752	0	666	301	379	279	323
331	318	548	334	98	378	355	209	264	304	506
370	577	571	573	272	317	566	332	668	282	464
325	695	506	480	307	373	260	497	341	371	260
369	694	185	518	330	497	175	355	594	584	610
605	582	626	336	615	169	584	803	602	718	574
715	587	605	142	616	163	607	217	287	731	731
319	626	631	653	290	500	207	456	291	464	492
481	231	303	601	612	490	172	248	324	376	610
266	212	262	360	245	71	119	247	332	285	161
225	116	443	467	447	439	440	469	432	448	460
519	548	394	713	731	406	672	638	695	661	715
405	0	168	706	663	673	236	466	216	442	481
446	510	422	472	0	322	285	483	565	0	391
360	384	125	144	219	291	585	286	134	287	17
310	387	427	252	348	366	535	318	308	320	70
315	0	239	319	115	431	222	229	394	291	485
252	759	1	259	334	1	333	279	496	331	273
496	1	438	302	313	258	364	355	723	619	0
7	236	343	396	220	552	1	359	517	690	555
272	458	359	259	428	160	383	0	595	212	522
101	534	634	441	908	303	149	386	166	0	658
295	999	518	180	144	322	609	593	563	138	461
675	458	0	509	179	449	676	273	679	346	649
943	655	179	720	347	145	147	199	231	702	670
318	208	296	533	531	625	345	557	544	253	33
175	185	524	466	763	531	293	429	512	447	511
601	450	555	504	498	466	338	631	333	465	537
635	605	202	513	664	0	679	1	690	683	846
299	478	207	48	22	216	219	250	156	136	



499

1848.6_1313EC75	292	298	209	311	314	307	334	209	568	312
242	338	354	352	384	373	309	373	279	392	275
431	301	442	285	233	425	385	327	556	406	567
545	560	485	441	594	245	541	363	341	297	285
311	320	505	271	248	379	379	250	316	292	405
347	609	582	594	305	287	579	318	654	288	461
306	667	526	469	310	353	333	496	356	361	378
308	366	290	414	327	408	210	492	426	535	581
567	510	558	235	554	167	679	574	674	629	496
620	679	707	158	695	157	708	272	298	636	643
309	682	682	651	343	437	362	473	280	490	490
439	266	279	583	547	341	302	258	305	432	458
337	336	197	312	318	266	164	288	246	252	307
314	285	430	473	425	420	438	480	444	443	392
377	481	340	610	609	380	559	466	581	554	598
391	239	301	548	541	563	187	322	135	290	362
282	278	300	336	198	244	348	387	465	253	335
401	349	207	251	284	334	571	222	327	333	159
317	321	486	194	394	336	272	374	437	281	300
318	251	348	466	322	305	294	334	446	59	430
187	613	175	231	310	134	305	294	433	251	223
400	0	431	241	344	291	357	340	514	606	7
295	127	331	371	272	592	268	405	501	685	491
389	272	254	282	403	310	339	185	440	314	518
281	484	539	352	478	285	277	328	220	255	580
258	518	999	309	275	332	575	371	520	124	720
378	640	190	709	295	360	682	156	682	346	643
512	542	280	579	343	282	290	339	261	553	453
471	231	334	672	644	604	413	455	547	315	293
192	327	472	467	541	462	267	432	449	457	588
331	305	488	560	501	490	431	556	284	411	394
471	448	188	451	523	132	516	16	538	539	503
302	384	295	388	276	364	248	389	344	286	

500

1850.9_1274EC11	248	179	103	273	282	327	225	206	326	181
233	402	200	211	209	262	224	233	155	222	216
345	364	412	282	200	286	214	209	317	242	263
292	295	268	266	305	156	278	292	245	206	242
214	176	285	187	134	229	254	259	264	231	222
240	299	284	297	224	286	286	261	284	248	447
256	328	446	453	232	316	250	444	337	294	262
224	246	219	296	213	332	231	266	288	322	301
318	303	285	195	289	202	338	303	330	304	288
309	342	339	172	336	203	322	246	219	313	310
235	286	285	284	255	208	250	345	215	342	235
230	264	295	294	266	241	229	237	256	341	287
236	248	257	237	215	261	164	179	306	298	209
217	235	280	319	295	299	283	317	286	290	290
291	290	286	286	280	276	291	254	294	288	308
291	150	761	279	277	271	285	259	35	231	283
213	14	232	293	164	197	334	308	280	191	269
175	195	179	135	322	225	357	159	143	395	105
147	192	201	162	204	164	112	397	327	236	285
157	127	267	311	199	211	229	313	196	36	247
284	305	34	15	271	5	158	181	257	245	179
201	0	290	184	265	193	209	115	254	301	62
223	210	320	109	226	327	138	273	319	335	344
172	73	136	218	181	204	253	132	316	250	185
161	295	333	181	259	181	200	274	137	10	325
271	180	309	999	198	220	303	232	254	31	316
0	178	142	283	198	250	326	229	334	206	300
308	303	189	302	163	587	127	790	295	282	228
294	82	88	305	300	305	253	230	298	564	548
287	752	277	200	222	332	127	252	237	282	322
215	270	284	270	291	312	447	286	10	197	263
183	253	61	218	271	50	259	107	270	230	260
222	259	316	389	395	318	291	377	324	397	

501

1858.1_1313EC36	337	343	195	372	364	318	374	163	226	283
266	304	554	382	204	232	348	204	218	361	307
315	212	266	516	247	250	484	356	287	375	275
286	245	198	201	212	209	270	444	298	383	310
402	606	274	246	208	344	424	253	335	715	221
309	215	219	212	357	294	214	285	199	257	213
277	200	215	214	307	222	651	209	187	165	397
174	197	615	176	221	251	208	303	219	251	200
212	226	212	269	234	248	218	194	220	173	229
186	217	193	212	219	211	214	616	725	195	198
210	179	180	181	275	213	249	238	241	236	176
189	282	206	191	188	159	212	648	279	349	162
257	301	259	196	334	676	201	322	323	287	172
240	566	193	210	213	238	207	249	278	270	227
172	163	199	181	176	204	185	159	193	204	200
214	157	188	146	193	185	200	196	41	190	219
136	68	189	156	181	166	253	197	186	180	341
287	241	169	678	298	374	257	144	244	327	168
611	189	262	167	214	279	131	272	324	220	319
265	570	340	317	358	217	443	451	179	98	213
328	221	181	278	332	299	426	565	299	279	194
153	0	180	244	376	445	274	458	145	256	179
257	2	324	206	337	167	319	314	209	196	278
184	179	291	318	202	672	215	446	153	406	209
585	264	227	74	163	203	606	152	225	198	280
175	144	275	198	999	103	214	164	200	111	222
0	180	127	179	736	219	173	151	184	275	255
156	201	728	244	139	252	430	213	637	223	121
207	10	624	250	186	383	506	394	391	249	255
212	219	434	184	145	192	200	163	136	194	243
172	176	221	324	309	265	283	175	108	184	221
176	224	18	197	185	206	161	75	196	201	145
208	176	253	245	223	228	140	240	233	205	

502

1868.5_1274EC17	208	225	190	6	234	11	240	193	271	6
61	116	358	254	308	355	198	248	278	282	159
175	187	244	148	234	308	302	226	333	269	327
342	336	311	345	333	135	267	14	235	197	120
187	252	331	314	82	255	307	139	233	152	344
208	265	368	329	205	188	350	311	239	281	256
294	287	177	251	235	268	201	201	238	276	191
217	325	155	243	263	331	226	185	290	335	319
379	318	295	281	295	153	316	229	341	231	336
240	290	261	174	226	141	301	109	181	273	266
167	297	309	293	204	222	2	332	233	349	253
256	88	0	250	230	304	94	191	171	189	221
199	140	184	172	150	90	159	238	247	153	241
141	68	276	283	246	287	243	275	251	263	296
305	277	233	231	239	159	247	239	274	268	278
253	161	125	262	243	248	128	225	80	190	226
182	191	211	305	236	109	203	202	216	221	234
207	289	163	201	10	240	268	175	190	191	4
358	317	320	490	198	255	216	288	263	207	4
236	121	186	277	1	295	239	175	335	29	302
0	292	59	233	361	1	239	121	341	287	83
255	1	238	193	185	160	241	142	325	335	103
212	79	185	261	93	293	273	191	344	288	417
131	307	193	182	233	157	285	180	301	188	319
0	258	211	309	240	322	199	323	273	74	233
485	322	332	220	103	999	408	214	292	92	153
7	290	134	326	34	269	285	213	299	239	299
271	240	102	287	353	142	170	161	104	272	246
94	252	286	295	344	250	0	281	308	205	124
5	202	253	176	220	233	110	271	294	228	311
270	284	259	243	226	268	231	227	21	306	239
211	283	160	278	225	172	205	199	238	302	228
248	256	226	218	216	170	63	240	168	155	

503

1869.1_1313EC75	272	277	41	327	312	293	307	241	629	226
249	321	309	373	383	433	324	357	408	338	328
432	241	479	297	276	390	345	330	523	430	505
502	491	416	551	822	38	743	394	314	260	283
328	345	550	300	222	357	291	225	310	283	493
333	921	933	936	275	312	924	315	850	255	448
325	820	451	454	260	356	248	478	360	366	281
393	409	247	397	322	421	188	439	445	736	966
960	762	945	302	910	124	600	605	640	790	737
788	586	608	49	637	97	618	211	282	737	740
290	689	706	819	346	459	212	430	313	438	502
483	221	315	664	626	463	242	216	333	397	598
332	318	232	334	263	221	50	324	249	282	133
284	199	426	513	455	432	442	481	450	449	413
465	605	451	601	605	439	578	526	794	595	772
444	29	280	625	559	572	200	432	331	537	436
496	464	500	524	43	406	338	515	525	33	361
400	354	53	185	265	307	638	271	201	332	85
314	413	507	215	325	371	310	379	447	240	268
296	211	236	349	337	395	265	292	336	245	566
178	767	118	271	273	28	297	232	512	313	226
413	0	440	237	307	270	346	319	622	910	0
245	187	369	430	243	757	248	446	583	824	528
347	373	220	229	453	223	355	118	616	287	698
196	605	615	490	505	285	236	388	186	143	636
226	609	575	303	214	408	999	379	951	117	591
253	528	155	588	259	408	713	193	731	389	710
560	658	193	542	326	254	229	300	216	515	627
478	282	321	581	613	652	405	496	654	282	302
253	293	675	504	556	592	293	414	629	450	589
400	349	587	623	583	500	453	617	318	516	437
527	478	244	407	582	72	505	214	563	558	551
300	465	276	347	265	357	225	338	258	323	

504

1877.4_1274EC17	189	245	6	237	250	239	218	227	365	136
306	275	228	221	214	217	225	236	159	319	502
347	156	287	182	173	307	284	217	311	277	259
297	314	342	345	464	6	444	245	327	280	280
277	243	334	245	172	269	257	196	196	232	261
274	388	385	385	205	283	385	269	437	264	382
290	397	376	382	230	300	206	379	239	248	181
284	512	219	314	231	323	162	265	379	340	353
349	322	344	178	348	137	349	746	360	437	317
438	359	378	25	379	129	367	242	220	479	481
235	346	350	396	282	329	200	289	273	286	286
325	160	264	271	328	291	224	267	246	284	394
249	259	207	245	179	93	27	234	273	249	84
225	102	319	333	324	311	302	348	317	353	276
318	363	269	447	489	292	471	398	456	485	443
289	12	209	514	500	509	198	329	201	296	334
319	283	296	313	76	229	224	298	391	13	253
209	186	122	189	251	218	388	255	101	265	333
203	201	282	154	207	304	426	304	296	267	250
198	99	228	266	261	226	192	313	302	6	350
282	440	178	192	292	246	306	223	268	263	239
298	0	236	267	356	222	241	197	517	362	160
192	242	283	242	256	341	28	321	310	436	400
319	98	176	124	273	194	300	116	369	168	309
120	324	314	341	618	269	231	228	208	3	463
189	593	371	232	164	214	379	999	362	111	231
551	288	198	346	149	356	375	166	380	249	464
636	323	185	574	300	172	48	224	220	570	397
271	74	111	344	347	369	257	258	281	234	180
254	218	296	398	611	372	252	288	379	291	155
432	232	397	265	309	359	227	456	276	242	318
387	456	217	319	418	41	553	79	498	507	581
288	368	218	251	219	228	174	246	247	114	

505

1879.6_1313EC75	287	296	60	324	309	278	301	270	585	259
283	293	292	361	345	371	307	312	311	337	318
379	229	435	286	243	345	317	327	496	412	474
485	472	367	505	784	62	700	393	311	246	308
268	312	545	337	212	335	279	220	371	258	448
332	864	889	893	280	306	884	326	846	248	426
333	792	425	432	251	365	240	441	360	333	261
358	353	230	354	292	403	189	429	428	716	921
930	740	954	280	952	131	575	546	610	744	722
721	576	598	108	629	82	602	215	254	679	682
297	677	695	815	336	433	201	411	282	418	469
466	225	302	630	593	405	232	192	317	401	567
301	293	278	314	229	210	109	354	260	290	141
261	172	406	529	448	416	417	457	420	441	412
402	565	436	563	573	441	549	502	782	574	770
438	97	227	592	527	534	204	428	330	524	431
471	449	494	513	111	337	293	474	498	55	357
392	358	150	143	280	301	601	233	194	344	88
242	383	469	223	305	344	312	360	398	168	283
232	196	238	345	325	295	235	297	241	212	516
183	745	199	244	235	32	226	193	499	320	218
359	0	358	213	296	226	331	291	582	868	41
263	147	365	390	305	726	125	399	543	804	500
286	245	259	237	424	206	313	129	609	238	674
153	560	595	464	459	242	186	307	164	114	628
156	563	520	254	200	292	951	362	999	140	542
266	523	124	567	215	367	702	240	722	351	671
545	628	183	525	316	215	196	253	204	480	595
455	321	300	579	616	631	410	448	659	249	262
223	247	707	485	531	604	262	381	610	426	554
308	268	566	647	605	486	393	585	352	455	405
504	470	247	377	546	85	489	91	528	529	527
268	436	204	294	158	309	173	291	183	295	

506

1882.4_1160EC15	179	192	120	179	219	46	134	215	189	106
218	34	119	134	202	139	221	153	44	193	165
142	143	148	101	135	49	120	114	91	190	20
80	96	213	210	118	91	140	154	122	171	211
125	82	38	106	51	261	189	219	231	29	219
238	176	173	173	229	60	183	247	113	204	147
204	152	195	157	183	272	141	188	188	201	154
209	212	197	187	251	287	240	151	204	260	147
186	150	164	1	137	676	109	144	153	155	188
170	95	70	141	120	272	155	235	143	145	165
225	120	104	149	269	170	111	168	228	143	62
159	282	269	116	138	171	216	206	275	226	221
240	176	296	287	256	57	106	84	282	227	134
247	61	214	266	230	257	230	265	285	271	248
243	132	270	160	177	363	150	142	224	232	213
330	59	2	180	135	125	253	192	139	132	215
161	63	235	135	58	130	236	190	213	60	125
90	159	216	2	28	134	54	101	52	39	190
1	190	54	4	143	68	0	2	110	0	119
2	6	85	137	156	225	43	200	145	0	195
135	190	1	4	94	2	143	113	26	149	81
203	0	156	0	119	179	267	150	52	166	2
139	168	70	0	0	86	0	87	32	40	217
13	2	102	48	42	59	42	33	167	80	38
2	196	74	119	127	10	134	225	209	1	114
118	138	124	31	111	92	117	111	140	999	101
220	124	144	28	130	105	138	125	99	241	114
140	47	36	133	100	121	7	62	65	65	204
118	0	66	168	104	78	56	60	44	222	88
78	59	35	128	1	197	236	2	140	76	1
61	180	137	153	107	176	116	147	16	2	90
110	227	1	49	218	25	1	16	99	45	108
220	17	127	141	153	103	152	153	111	146	



507

1882.5_1274EC11	266	295	101	289	281	242	294	208	495	229
264	369	306	323	314	389	239	340	212	361	229
392	291	436	292	186	383	309	288	489	380	477
476	462	413	334	596	96	532	353	290	305	287
250	367	575	366	178	339	348	244	291	343	414
293	573	540	542	254	325	533	298	666	290	418
302	697	461	428	279	383	272	450	337	349	340
299	291	270	417	287	430	215	489	408	544	586
586	512	595	224	591	190	690	491	696	630	518
636	693	701	144	709	141	704	282	302	628	627
304	672	670	642	278	400	321	465	325	468	540
407	275	307	668	583	372	276	275	343	463	453
303	363	256	337	345	236	128	243	283	249	265
309	228	408	469	414	407	412	474	406	459	424
396	504	390	592	593	461	547	437	568	550	574
421	78	323	514	508	511	236	330	64	330	346
230	106	288	353	122	220	370	379	490	48	313
368	296	202	233	250	294	534	196	135	383	191
246	317	442	177	330	258	233	373	421	197	321
237	209	228	372	316	238	321	301	317	90	330
255	631	202	194	231	8	231	273	484	378	232
321	0	401	237	367	301	290	247	483	599	40
254	76	370	358	247	627	293	351	472	699	519
375	170	176	280	390	284	305	159	437	320	545
267	490	574	276	425	217	283	281	222	250	562
242	461	720	316	222	153	591	231	542	101	999
0	674	140	655	262	279	687	162	708	301	620
457	590	236	608	277	330	187	355	237	573	460
446	138	372	680	707	650	459	437	582	354	329
178	347	528	462	488	486	283	365	468	423	545
340	319	547	554	508	529	487	541	304	323	414
424	444	261	370	496	123	477	240	499	505	472
337	367	368	422	386	382	245	418	332	378	

508

1888.7_1313EC36	0	279	0	0	0	0	2	243	284	0
0	5	1	0	0	0	0	0	0	207	203
255	0	275	0	0	21	3	1	7	4	1
7	7	246	285	443	0	429	2	12	2	0
0	0	15	8	317	232	9	159	2	1	342
141	356	350	401	4	9	388	182	415	220	399
177	410	406	393	225	192	0	387	0	177	4
174	541	1	366	174	266	139	0	325	334	392
375	318	392	29	386	129	346	469	364	313	317
308	244	260	0	268	139	266	119	280	370	369
285	412	399	398	148	410	11	214	221	214	18
398	15	319	360	392	340	220	0	136	297	394
259	214	204	311	183	0	0	3	199	25	0
207	0	214	203	212	224	211	231	148	230	229
277	317	16	391	430	133	409	405	421	419	432
192	0	0	444	411	424	140	270	247	220	279
326	296	209	263	0	337	209	291	365	0	0
22	2	146	0	0	2	257	238	0	6	0
1	0	17	0	0	329	256	2	203	15	0
213	0	0	0	5	0	2	6	0	0	349
0	357	0	0	6	0	0	0	7	4	15
424	1	6	0	28	11	145	0	140	394	0
0	205	11	8	0	222	0	0	25	284	229
7	0	241	0	249	1	5	0	22	5	5
1	318	343	0	723	0	14	1	163	0	396
3	675	378	0	0	7	253	551	266	220	0
999	0	0	20	4	229	429	254	405	303	243
717	47	1	424	1	203	19	0	12	173	383
3	0	6	209	150	34	10	317	3	0	0
24	0	22	21	458	85	223	86	254	220	0
470	284	224	232	179	23	0	345	23	0	300
382	373	0	116	402	0	209	0	432	329	633
30	33	148	1	0	0	0	212	0	0	

509

1889.9_1274EC17	227	172	144	273	259	267	316	243	526	246
244	281	282	277	364	398	300	316	302	279	288
317	231	304	221	262	392	322	232	537	275	534
566	565	408	456	555	226	496	305	323	261	301
231	292	512	271	153	281	310	197	272	227	384
300	528	550	547	271	216	529	275	625	213	430
275	648	484	429	268	304	233	465	379	292	274
284	349	235	473	309	384	140	397	381	497	528
521	483	496	215	490	169	921	515	920	544	471
551	923	920	202	874	95	881	166	236	574	557
235	798	787	672	250	407	208	488	188	492	604
438	315	237	678	608	323	191	166	281	367	478
213	285	224	280	253	260	166	288	261	248	188
235	230	430	422	460	446	442	451	450	431	374
447	469	329	634	627	381	583	417	550	564	543
372	180	143	515	525	537	191	367	174	335	371
372	228	324	348	197	184	299	324	417	190	256
334	321	109	175	245	316	514	243	258	271	136
304	381	428	231	354	311	289	369	310	245	195
326	212	355	368	164	369	246	252	367	160	419
148	591	161	205	291	23	235	192	442	264	216
384	0	374	246	276	264	282	290	488	584	32
296	178	260	321	300	539	202	276	487	648	439
329	313	257	257	411	199	307	192	480	246	509
220	423	515	311	428	183	184	285	228	270	507
328	458	640	178	180	290	528	288	523	124	674
0	999	0	938	207	331	789	202	768	261	523
462	626	222	629	276	210	263	243	188	657	511
374	193	285	782	865	653	397	440	561	212	205
185	231	456	478	412	446	302	430	380	460	514
372	394	427	484	452	458	383	464	305	370	386
409	377	181	466	442	3	473	1	514	480	466
278	359	265	354	238	275	194	333	255	265	

510

1892.7_1313EC36	145	188	0	165	219	123	206	192	137	1
264	171	201	132	181	227	206	159	0	234	190
192	176	143	137	126	164	199	240	138	236	129
148	137	130	104	111	0	141	109	214	245	179
154	140	23	69	182	251	182	253	209	141	120
251	154	172	173	250	85	181	197	118	183	169
183	127	155	165	191	209	168	149	184	208	170
196	152	134	75	202	222	281	200	201	197	131
136	152	149	1	138	223	161	187	169	173	146
171	157	160	140	141	186	176	297	138	160	175
230	125	129	117	386	145	228	196	291	164	162
115	216	280	137	114	92	213	257	412	152	108
238	163	199	244	189	126	84	165	173	158	110
218	87	190	204	184	199	181	217	245	263	177
184	182	188	146	148	238	152	176	158	204	176
242	69	81	177	154	156	257	172	3	195	199
173	6	190	144	126	180	194	237	181	65	182
59	189	481	133	137	206	146	192	0	109	0
101	0	142	0	0	157	258	130	246	1	126
136	110	66	194	219	0	90	136	1	0	108
210	102	0	0	211	149	0	156	129	47	220
0	689	136	0	70	108	264	226	173	148	0
201	135	146	0	4	174	98	124	113	99	170
3	0	0	132	129	171	131	140	158	156	3
87	162	120	2	1	126	193	165	155	0	129
172	0	190	142	127	134	155	198	124	144	140
0	0	999	181	108	208	89	118	88	399	237
157	140	138	132	9	165	170	162	197	20	42
2	0	180	174	98	154	1	0	10	163	97
7	149	74	153	4	159	45	138	67	145	0
2	106	172	157	144	166	210	89	2	0	138
2	185	136	151	160	130	0	167	132	1	97
161	73	186	200	171	172	249	199	231	25	

511

1909.6_1274EC17	270	251	0	362	315	288	330	259	582	263
279	268	318	271	393	417	291	277	368	306	365
361	180	377	256	208	387	323	270	555	355	526
565	561	374	493	610	0	561	297	345	304	304
304	255	513	282	168	320	322	214	278	284	404
290	566	583	585	296	258	562	307	664	274	434
288	677	493	432	264	320	303	472	356	345	252
309	400	251	468	329	420	178	445	425	530	573
574	507	533	312	528	146	915	545	903	571	513
576	909	918	50	866	99	885	180	260	602	586
312	817	807	705	273	415	211	503	227	501	632
460	328	236	678	622	348	246	206	339	342	517
279	275	247	282	292	178	45	317	295	269	170
266	184	421	450	452	433	436	450	470	456	381
455	509	350	666	665	377	629	472	613	637	607
397	0	317	575	571	586	232	332	164	354	354
313	271	328	348	213	170	312	358	467	0	367
347	385	138	150	268	330	589	240	230	283	16
344	395	482	209	360	328	353	334	348	237	169
382	1	352	409	222	384	227	263	324	213	485
241	621	6	208	317	4	316	220	454	267	229
354	0	373	232	280	225	292	305	534	622	0
215	146	302	334	251	602	110	354	508	688	461
334	404	323	209	386	156	326	45	470	231	512
202	452	587	371	462	263	132	382	127	331	505
326	509	709	283	179	326	588	346	567	28	655
20	938	181	999	206	368	802	237	786	294	564
488	633	219	658	270	245	177	300	188	665	511
370	198	286	820	888	671	405	482	554	278	225
196	299	494	517	507	460	285	406	416	430	541
394	426	412	518	475	444	403	497	247	411	413
459	421	173	535	518	2	542	3	564	551	542
311	401	237	276	181	232	172	295	244	240	

512

1915.4_1274EC17	333	311	208	376	372	275	342	170	267	275
273	295	480	384	245	272	353	231	264	329	333
385	210	275	464	288	262	436	380	287	437	241
294	264	251	221	244	174	285	398	325	422	373
514	547	304	256	161	411	493	264	320	635	242
340	250	252	245	407	307	247	301	278	258	227
298	247	223	228	304	252	532	213	256	218	519
215	205	514	225	231	316	204	333	245	290	222
230	243	225	311	241	257	254	253	256	242	237
257	241	236	202	257	172	254	494	948	270	268
209	207	206	234	322	225	267	262	273	257	208
221	326	163	236	211	175	220	492	283	359	246
282	326	274	202	406	579	198	363	335	329	156
256	553	252	271	270	290	259	305	311	317	293
269	224	266	247	243	255	254	223	255	266	261
283	161	168	231	259	252	206	202	110	163	225
191	107	168	172	163	199	282	224	231	164	364
306	263	144	485	279	342	297	131	272	326	144
512	207	243	175	225	297	229	274	392	227	325
266	538	326	347	404	270	468	409	221	153	202
347	242	211	325	365	343	533	561	292	309	178
200	3	208	233	365	485	324	421	196	255	184
293	76	366	233	323	299	366	341	255	258	272
198	217	297	340	211	556	223	431	198	488	186
448	281	257	141	188	236	498	235	226	234	386
154	179	295	198	736	34	259	149	215	130	262
4	207	108	206	999	191	210	173	222	333	293
183	208	647	258	175	235	427	231	552	251	219
252	35	508	276	236	377	406	395	396	243	252
255	213	358	218	224	194	216	223	225	243	248
214	247	271	365	366	316	312	231	134	213	284
212	261	141	219	249	185	222	50	262	234	220
289	232	281	276	243	267	154	270	265	226	

513

1920.1_1313EC57	332	260	14	363	347	268	297	285	527	264
325	225	311	344	519	549	329	443	497	362	432
365	167	342	254	235	493	290	278	449	330	414
402	395	455	536	482	7	401	279	351	287	336
390	261	433	323	218	464	389	268	305	248	460
326	370	387	390	324	299	381	369	425	333	339
320	432	347	342	322	484	255	334	494	388	312
353	405	304	414	419	457	209	395	462	361	383
396	437	372	342	422	140	428	479	429	446	429
426	428	440	92	415	180	434	274	232	493	493
286	374	377	374	339	423	185	531	247	528	443
437	231	136	407	435	443	239	247	365	348	403
269	255	271	250	282	121	129	311	254	230	214
248	141	375	364	348	367	357	405	368	401	364
416	452	405	461	441	343	475	407	413	435	419
360	141	196	450	474	450	266	379	129	322	367
318	349	325	316	97	185	334	333	391	151	385
439	499	217	215	259	297	541	245	207	281	193
308	518	424	251	514	391	417	421	396	347	104
369	165	244	385	139	575	334	249	473	265	530
267	485	274	292	372	25	400	266	412	390	206
494	137	477	333	322	279	353	382	505	373	257
174	97	296	435	323	451	48	297	389	463	477
281	476	381	212	259	161	407	115	448	303	390
51	373	444	400	378	405	96	501	152	43	466
301	449	360	250	219	269	408	356	367	105	279
229	331	208	368	191	999	419	298	428	381	490
387	461	223	409	491	227	157	199	230	438	428
323	277	351	403	358	469	15	411	459	258	138
220	223	376	377	361	442	247	424	360	423	414
462	376	426	395	398	396	423	471	230	445	406
441	373	211	444	445	103	439	135	489	494	445
369	408	315	273	368	340	295	314	323	185	

514

1924.2_1313EC57	281	264	9	312	318	247	330	240	629	246
273	324	269	304	382	423	278	310	360	340	367
411	225	482	223	284	395	300	319	550	386	546
534	539	389	473	761	6	677	311	359	293	325
322	279	606	309	194	343	296	212	243	284	483
310	661	664	667	288	313	658	305	823	236	458
282	845	493	464	254	307	244	482	367	351	256
353	446	223	482	351	438	187	416	456	617	688
685	631	695	310	690	122	839	621	866	718	604
718	839	849	86	829	117	814	212	249	705	704
312	966	965	899	309	431	201	540	315	548	641
420	296	275	765	718	413	254	205	293	378	602
330	315	286	289	271	121	75	295	288	245	183
273	155	445	503	448	445	456	466	428	460	427
494	582	394	697	716	408	668	541	702	666	697
405	92	320	682	606	621	215	431	278	462	435
405	445	454	483	79	292	298	450	529	87	345
362	417	85	183	234	330	642	173	206	328	124
270	441	511	244	345	340	368	387	397	326	203
259	100	220	342	272	362	240	227	331	223	481
222	732	99	263	296	199	327	225	565	294	226
408	0	450	248	277	236	315	292	642	684	38
224	143	361	391	259	706	218	392	586	851	507
313	427	334	207	461	169	347	24	573	267	598
138	538	662	393	586	269	150	352	161	217	631
308	676	682	326	173	285	713	375	702	138	687
429	789	89	802	210	419	999	209	972	327	632
624	739	186	715	326	248	144	315	238	716	611
409	204	322	847	870	776	433	521	625	288	215
195	321	599	583	616	541	287	443	534	465	551
420	422	546	572	538	521	425	607	301	469	441
527	437	216	532	615	132	561	66	620	612	633
310	459	263	314	297	292	259	325	215	263	



515

1924.5_1313EC16	190	165	226	260	289	173	160	169	291	145
178	155	221	187	253	293	200	211	302	223	235
180	130	186	212	269	220	254	254	251	294	264
237	236	235	264	242	230	240	126	138	186	191
235	196	269	351	56	319	235	184	265	222	214
299	171	194	168	147	185	167	223	219	180	154
198	223	178	161	175	224	152	162	206	170	220
175	232	184	180	193	246	208	187	271	258	183
200	177	198	247	183	197	245	187	243	186	183
210	224	195	226	214	191	224	183	219	204	180
233	201	202	221	292	229	54	225	192	222	218
230	186	103	179	178	264	217	193	200	221	211
243	196	165	150	109	155	223	300	215	223	196
205	153	172	221	195	205	182	240	204	271	205
214	186	185	183	169	191	203	208	232	219	224
150	215	143	176	187	183	167	223	190	253	236
197	75	199	216	218	198	181	233	165	229	303
318	331	168	0	131	160	320	180	200	191	2
352	273	235	272	287	277	228	215	258	152	104
185	279	185	204	226	219	224	182	318	155	205
86	194	0	176	245	0	247	70	271	380	57
215	196	170	235	205	172	332	226	267	207	62
80	136	215	246	123	250	69	249	250	236	252
77	311	365	70	158	219	190	175	250	240	147
0	202	185	214	206	227	144	203	184	112	222
231	273	156	229	151	213	193	166	240	125	162
254	202	118	237	173	298	209	999	211	280	224
186	234	93	212	217	251	170	195	168	266	191
130	137	242	253	225	200	62	217	228	255	229
126	193	167	195	246	188	238	155	216	131	277
212	216	207	196	234	215	224	188	85	252	148
202	190	123	293	204	1	199	48	172	223	166
175	161	247	232	170	217	200	223	153	102	

516

1931.9_1313EC75	287	277	12	339	340	261	342	259	663	269
301	361	282	331	419	432	282	305	375	351	380
429	210	484	254	233	418	301	341	587	413	571
559	546	406	503	772	9	679	334	350	290	330
318	323	604	321	208	354	308	213	266	297	482
328	704	703	709	294	327	697	318	840	263	464
313	860	519	467	283	328	257	491	396	365	271
364	455	238	493	363	461	197	427	466	633	703
697	654	717	318	704	117	838	634	861	730	626
731	834	849	65	833	146	815	212	256	718	718
335	943	955	911	330	442	210	546	314	553	655
455	326	284	788	741	406	276	209	319	372	617
330	321	283	317	329	130	62	309	292	249	205
294	158	442	515	448	442	459	469	430	480	434
497	585	401	700	719	420	670	534	717	671	708
416	67	326	690	610	628	228	424	290	451	428
443	450	443	493	58	314	313	481	534	61	370
369	434	100	191	250	342	681	220	211	352	21
288	452	507	212	339	351	382	389	420	299	222
290	110	243	352	305	380	241	251	369	194	513
226	746	112	250	293	3	333	233	549	304	236
423	0	459	285	305	253	333	329	650	698	47
267	151	377	441	206	738	188	413	594	867	524
349	439	325	221	489	191	364	37	581	280	602
145	567	689	454	589	289	159	367	166	141	645
305	679	682	334	184	299	731	380	722	99	708
405	768	88	786	222	428	972	211	999	362	655
625	771	210	721	317	253	151	333	251	722	621
423	208	325	826	840	800	442	558	648	303	241
208	327	625	596	620	549	300	444	552	471	597
430	418	548	618	586	524	457	602	311	479	478
527	464	237	541	614	166	568	80	621	613	642
306	448	260	317	235	305	201	333	229	291	

517

1938.9_1274EC17	317	320	126	486	387	301	378	271	424	382
243	366	361	397	285	366	371	286	367	368	556
568	192	406	357	240	311	346	690	305	662	298
323	306	308	303	367	113	335	342	538	382	266
236	354	403	670	231	358	359	286	343	308	333
722	348	357	358	419	333	353	240	396	270	293
246	389	310	298	249	352	331	314	294	339	318
297	253	322	253	332	315	228	280	298	375	379
392	356	380	366	375	239	340	356	353	390	358
385	335	331	66	346	202	329	306	360	369	367
305	337	336	369	944	283	220	282	331	277	284
274	237	252	349	344	283	308	276	362	336	306
332	274	280	328	298	200	75	569	270	340	160
322	228	304	309	326	299	292	329	321	346	296
316	349	322	320	322	327	329	329	349	325	326
360	94	186	322	337	334	223	295	103	290	320
268	264	283	319	97	227	292	303	292	94	469
402	364	273	294	321	378	431	270	264	397	45
314	301	294	291	322	330	538	306	600	219	239
286	164	315	361	613	339	341	431	347	250	310
281	359	220	147	481	127	264	235	333	623	209
245	338	276	227	344	322	709	347	317	377	205
271	100	389	317	321	398	194	414	325	400	342
109	301	278	282	314	309	306	173	465	299	335
189	379	408	285	353	324	300	309	255	5	420
253	346	346	206	275	239	389	249	351	241	301
303	261	399	294	333	381	327	280	362	999	376
286	366	289	345	331	224	192	206	310	354	314
395	138	296	323	316	360	218	355	346	233	247
288	182	359	359	360	353	219	287	359	256	297
305	276	375	345	297	300	345	351	145	328	287
318	324	111	297	336	174	351	103	323	330	290
253	311	237	248	238	299	171	289	270	257	

518

1956.6_1313EC75	319	358	175	363	345	333	358	228	571	271
310	379	334	400	370	429	320	405	360	392	408
479	254	476	312	301	436	376	377	516	471	497
495	496	456	484	723	236	673	441	367	341	360
296	357	572	373	240	370	388	241	337	323	496
367	661	645	645	334	354	638	327	743	292	482
332	727	512	481	294	447	294	488	358	378	368
363	451	336	431	339	498	214	426	457	616	705
704	627	683	325	691	150	630	653	640	793	612
792	631	644	203	654	168	642	253	318	788	785
316	589	598	662	363	510	284	536	331	539	529
502	272	271	631	610	486	293	232	394	478	540
357	376	260	326	360	280	197	358	304	307	271
319	273	470	494	476	474	469	527	485	468	482
454	774	488	788	788	510	763	705	772	755	771
509	210	316	751	743	748	224	381	158	386	394
352	343	357	381	234	293	393	410	732	213	368
443	419	212	250	318	358	584	231	221	376	195
294	388	448	240	444	350	389	424	473	311	298
304	234	328	411	373	387	403	393	371	184	495
249	710	230	247	328	27	274	253	524	377	240
419	0	442	297	461	337	384	352	615	687	60
277	138	411	440	373	691	240	486	574	756	616
357	307	287	289	411	299	342	213	646	366	627
198	550	663	519	583	267	320	376	232	196	647
377	649	643	300	255	299	710	464	671	114	620
243	523	237	564	293	490	632	224	655	376	999
628	654	253	628	388	328	249	336	324	614	627
537	262	317	578	564	667	388	530	663	370	367
246	344	615	508	626	590	312	466	617	463	593
453	341	720	557	559	503	503	824	401	534	480
747	551	253	586	753	132	707	116	773	760	684
381	579	375	422	372	383	255	420	341	354	

519

1973.7_1313EC36	259	329	1	299	342	234	284	281	587	220
297	314	277	283	343	371	272	291	304	385	515
377	203	423	220	231	429	283	225	444	345	417
443	429	361	440	714	0	646	314	348	293	296
280	291	471	309	207	371	340	213	219	311	452
362	535	527	531	252	311	524	316	625	276	425
312	651	463	440	279	359	236	453	319	360	250
324	697	179	460	281	475	185	332	569	543	561
556	536	587	309	564	164	563	800	573	656	532
651	567	593	57	595	145	597	217	286	684	685
293	572	577	602	273	465	232	433	308	438	444
450	223	325	536	561	445	241	222	321	365	581
291	269	248	346	255	113	94	244	326	302	159
250	128	414	442	423	418	432	456	427	438	426
499	506	365	670	699	400	631	604	663	632	682
379	65	283	660	638	650	226	448	215	407	457
417	469	384	447	2	335	278	456	552	74	356
333	367	111	187	220	284	584	289	141	296	15
260	396	436	216	290	351	550	343	337	340	203
266	100	215	345	217	367	240	215	327	186	435
212	707	98	284	294	2	282	225	439	286	265
421	1	391	288	315	289	340	327	709	574	0
218	225	331	328	159	551	208	373	454	660	523
309	403	344	215	377	189	371	0	542	252	495
141	486	570	436	922	241	186	363	156	2	625
233	943	512	308	156	271	560	636	545	140	457
717	462	157	488	183	387	624	186	625	286	628
999	584	163	743	297	205	148	321	196	719	643
383	191	294	527	507	566	298	508	485	251	228
226	296	487	437	783	507	287	392	460	416	407
575	434	514	462	458	464	406	604	318	421	495
598	598	201	497	647	133	691	3	658	659	856
287	450	250	258	237	278	248	307	168	277	

520

1999.3_1313EC75	287	298	167	338	348	251	320	240	599	270
334	375	324	386	470	512	295	366	519	364	339
465	225	496	271	253	446	358	322	533	392	526
547	553	435	535	678	192	671	342	354	301	332
324	374	712	309	220	368	309	228	261	324	680
315	586	590	596	277	310	584	339	685	236	441
333	697	492	449	235	345	337	464	377	376	277
351	477	253	464	390	491	190	364	512	564	621
635	576	620	332	673	146	654	611	658	711	569
713	644	637	179	664	164	644	249	258	774	776
339	706	706	698	345	534	194	543	324	544	807
606	292	288	903	930	670	249	231	342	372	596
301	342	306	339	322	144	180	345	265	263	296
296	155	388	437	395	377	380	447	415	490	452
414	505	370	614	624	405	567	485	616	582	619
402	251	302	594	540	558	275	427	127	427	432
403	380	413	435	252	275	327	431	517	287	363
419	430	48	228	261	320	635	231	84	384	261
311	456	622	232	450	362	365	444	463	476	229
307	8	268	340	296	435	294	274	414	161	500
241	742	120	292	311	4	328	265	683	325	211
437	0	477	317	296	252	354	339	638	630	1
222	162	343	460	267	668	150	398	543	768	486
319	421	269	235	400	223	361	49	533	281	749
130	518	630	428	559	347	148	451	183	86	583
274	655	542	303	201	240	658	323	628	47	590
47	626	140	633	208	461	739	234	771	366	654
584	999	204	635	299	286	142	331	271	627	640
387	125	443	703	680	694	395	531	580	309	293
216	318	544	531	609	504	305	390	558	435	622
459	420	527	538	564	484	508	574	316	536	459
474	439	155	460	540	75	534	50	570	591	587
289	449	304	311	269	308	221	348	232	313	

521

2002.2_1178EC16	343	334	146	296	329	330	355	179	263	233
342	282	621	370	191	269	303	201	202	329	319
289	191	253	612	276	320	541	341	276	350	249
285	253	205	207	206	166	262	470	348	366	303
286	664	272	238	170	298	337	265	359	729	227
286	247	250	243	320	319	248	316	172	289	238
326	187	229	235	327	241	733	212	255	186	322
198	221	640	235	229	294	214	287	241	235	225
197	212	246	301	240	236	244	233	246	215	208
213	235	186	156	204	185	199	679	621	222	228
203	191	193	187	306	219	287	270	285	270	172
208	270	172	199	186	169	244	775	250	346	202
267	318	270	201	325	594	141	255	289	281	163
286	563	195	219	211	235	190	225	248	295	233
206	176	219	221	207	213	218	160	235	235	230
226	145	143	176	230	212	215	188	169	208	248
220	181	190	185	192	177	327	191	206	153	292
300	301	96	747	294	355	282	216	236	311	261
668	231	232	252	213	293	158	304	332	242	336
274	595	301	354	303	240	444	456	246	89	217
297	224	178	210	352	297	272	522	289	298	158
203	0	174	342	393	333	272	408	191	273	155
206	114	343	279	351	215	297	364	277	176	287
222	242	317	284	274	780	209	450	183	334	195
603	252	215	154	177	157	643	199	262	204	285
231	179	280	189	728	102	193	185	183	36	236
1	222	138	219	647	223	186	93	210	289	253
163	204	999	241	205	242	541	205	701	232	197
264	23	745	294	222	378	558	472	430	236	262
234	188	383	241	184	177	270	161	159	182	280
160	232	212	318	287	253	338	200	180	207	218
178	249	176	231	217	221	230	150	231	216	188
261	176	293	298	262	330	210	294	321	165	

522

2023.2_1160EC43	296	325	129	311	296	294	313	229	540	224
292	357	322	352	345	364	274	310	294	384	565
430	207	414	280	242	428	329	320	478	439	480
477	493	377	433	613	120	565	367	391	331	328
305	307	558	508	248	369	329	240	252	328	429
381	527	510	515	310	320	509	329	647	281	397
302	664	459	404	275	345	286	426	300	310	282
286	637	263	438	283	464	204	364	461	556	527
526	505	541	343	527	157	702	756	681	596	524
601	703	707	81	645	142	676	242	299	649	647
298	663	663	689	330	440	277	429	323	433	540
431	341	257	599	604	385	290	217	360	421	537
320	385	257	316	317	229	79	315	334	285	195
316	256	384	435	399	393	404	430	395	441	420
457	484	397	702	713	414	638	481	634	646	602
387	79	286	633	637	636	237	364	150	336	370
298	332	320	353	78	203	312	362	480	73	333
396	395	130	249	272	313	558	223	184	356	157
283	349	443	203	331	350	557	358	375	266	282
274	138	258	368	335	343	320	323	322	131	444
228	676	201	245	338	25	294	236	521	494	276
356	0	424	296	413	321	364	347	691	543	34
275	169	373	349	287	594	245	372	454	701	508
362	341	278	251	386	273	348	161	471	315	468
202	483	560	435	694	238	267	345	240	157	626
264	720	579	302	244	287	542	574	525	133	608
424	629	132	658	258	409	715	212	721	345	628
743	635	241	999	290	248	239	304	285	954	576
447	187	295	654	698	590	352	453	509	289	279
198	293	521	517	746	496	327	385	480	380	433
504	414	510	497	472	467	409	558	299	410	453
511	441	197	569	557	129	676	212	683	656	733
317	418	307	339	309	317	236	342	266	318	



523

2023.7_1274EC17	258	210	164	257	309	269	267	462	385	225
240	254	319	242	354	342	242	322	339	306	303
286	155	312	260	284	308	275	272	317	285	296
330	329	289	355	342	181	281	266	307	232	323
254	292	325	257	150	338	240	185	304	220	323
338	288	239	236	304	366	239	590	350	561	286
569	370	284	280	542	652	244	305	401	524	220
544	394	253	315	270	427	196	267	370	308	353
314	284	321	218	331	85	311	393	300	356	311
350	308	302	204	304	176	313	155	207	387	384
235	224	227	301	333	268	226	414	235	409	313
267	255	178	314	304	267	176	247	255	360	338
248	206	227	220	208	151	206	219	275	133	168
229	136	470	539	482	467	458	506	489	485	500
530	388	318	350	346	368	339	352	348	358	355
341	227	168	338	350	345	182	273	109	326	351
221	344	327	335	197	176	297	308	364	189	313
305	421	143	156	228	267	363	476	74	286	84
306	355	314	246	386	325	377	277	307	196	147
244	116	235	305	147	383	407	272	333	189	376
150	359	258	243	343	0	274	232	318	228	205
345	8	341	215	344	254	337	406	343	293	3
172	234	346	269	281	339	57	247	303	373	561
212	301	215	305	311	258	559	163	349	218	309
43	411	316	131	258	572	174	301	172	148	311
363	347	343	163	139	353	326	300	316	100	277
1	276	9	270	175	491	326	217	317	331	388
297	299	205	290	999	155	148	211	251	304	331
469	485	244	326	260	284	120	255	318	185	123
127	183	294	288	307	588	267	465	236	517	316
456	547	400	269	288	454	315	383	177	321	539
375	522	417	344	361	19	319	9	389	383	373
678	500	299	285	250	316	99	326	265	177	

524

2029.2_1274EC17	288	337	275	294	307	267	279	228	277	198
285	338	217	273	233	281	244	261	216	326	197
357	375	389	272	243	303	231	246	305	285	235
299	269	254	222	255	311	318	286	299	282	277
253	239	249	199	181	344	281	300	335	242	225
275	300	283	282	263	296	284	287	247	250	356
268	280	384	361	230	347	259	377	350	297	325
251	278	283	264	245	388	301	273	292	334	249
296	257	255	105	249	294	306	280	319	285	250
313	302	272	277	323	315	302	275	257	331	328
262	238	234	229	286	255	254	307	261	306	254
243	266	288	238	234	206	282	220	306	360	229
274	322	305	288	290	319	321	171	339	218	386
275	284	304	347	331	344	311	367	350	390	327
285	246	224	295	294	350	297	246	275	318	295
291	312	608	258	290	266	270	245	174	219	269
169	9	255	210	307	237	423	304	299	321	257
238	292	349	196	258	279	289	190	178	329	194
165	182	242	129	268	171	149	342	324	145	345
158	167	259	323	224	261	286	342	135	106	204
256	253	158	96	237	16	208	224	238	170	190
180	88	262	179	286	234	243	284	257	289	156
285	157	305	157	245	314	225	328	272	269	379
192	164	199	332	226	251	215	164	262	309	143
178	409	299	176	272	181	238	202	258	183	368
304	145	282	587	252	142	254	172	215	121	330
203	210	165	245	235	227	248	251	253	224	328
205	286	242	248	155	999	216	616	325	269	154
277	13	131	340	281	287	189	273	306	816	747
278	606	314	268	241	298	145	235	143	262	295
200	220	307	345	371	258	493	281	128	244	258
216	328	105	245	284	65	204	304	258	225	204
272	208	480	521	493	437	413	489	455	427	

525

2039.0_1313EC43	259	336	198	327	325	260	344	142	143	266
320	238	367	330	200	197	297	212	208	326	287
305	168	156	325	208	210	364	254	290	290	142
297	232	194	163	180	223	199	275	333	290	302
328	466	141	219	195	365	349	215	293	410	178
252	277	276	265	303	292	276	304	149	220	227
282	169	237	228	239	242	390	232	248	143	274
179	214	482	234	174	315	199	245	266	316	258
242	305	284	259	238	269	264	198	266	189	302
197	273	256	210	276	197	278	401	439	240	247
151	191	182	178	270	248	236	230	197	233	190
253	294	182	200	155	105	92	369	287	311	162
206	279	281	206	309	462	197	205	325	272	220
183	434	252	308	310	301	277	310	339	320	231
197	190	158	238	245	235	243	197	261	283	265
243	181	37	184	251	259	229	161	78	183	203
141	106	198	147	175	89	301	194	214	176	231
216	252	178	303	246	344	125	87	206	245	261
327	136	200	223	207	218	150	145	288	28	247
149	375	308	248	289	239	341	364	165	160	116
210	197	58	158	292	10	330	327	212	156	195
114	155	123	263	334	307	175	435	153	280	214
115	92	315	160	245	85	191	225	137	121	286
240	110	234	281	199	475	92	327	128	263	133
342	257	128	47	183	108	508	112	297	172	249
192	147	290	127	430	170	229	48	196	7	187
19	263	170	177	427	157	144	170	151	192	249
148	142	541	239	148	216	999	195	403	193	127
79	2	317	296	239	296	297	291	293	225	240
150	168	349	302	184	241	216	247	173	201	127
114	146	178	356	337	243	215	143	89	192	207
159	258	77	212	212	76	154	133	213	140	100
186	73	242	258	156	183	118	213	186	114	

526

2048.2_1313EC75	261	256	200	305	291	350	253	210	315	171
	266	391	218	247	257	289	240	280	226	239
	368	379	404	295	222	299	210	238	336	243
	317	298	281	276	298	257	308	330	281	292
	248	220	266	220	150	262	246	270	288	236
	248	318	301	316	257	305	305	278	307	450
	255	362	440	456	258	348	238	460	346	296
	208	261	270	327	238	377	242	327	361	298
	334	335	285	101	284	222	358	350	363	311
	353	360	350	252	372	225	366	272	255	364
	231	318	308	305	272	261	268	365	247	246
	262	287	302	320	302	245	223	239	262	323
	253	282	275	269	250	279	253	173	352	305
	234	273	275	342	323	315	288	352	333	320
	314	324	279	341	337	337	353	299	323	318
	318	243	758	324	331	324	292	272	168	329
	155	8	270	281	260	217	362	319	323	281
	288	244	237	169	338	253	306	197	181	170
	122	187	238	131	260	185	165	400	349	345
	147	182	292	318	197	244	301	339	194	249
	242	325	170	42	260	14	211	195	235	151
	203	0	307	175	285	198	204	188	260	52
	241	172	327	131	251	307	209	270	282	362
	208	64	137	261	177	246	203	112	309	195
	167	316	326	162	278	146	242	257	188	347
	274	199	339	790	213	161	300	224	253	355
	0	243	162	300	231	199	315	195	333	336
	321	331	205	304	211	616	195	999	275	263
	309	30	111	378	301	283	252	230	308	569
	267	803	332	192	249	351	152	231	202	299
	224	265	320	312	317	297	485	334	10	294
	226	277	125	209	324	77	247	178	308	282
	272	249	410	509	439	407	353	426	377	461

527

2064.0_1191EC10	324	359	189	291	339	345	350	200	325	294
287	380	702	349	202	259	336	223	225	374	341
358	165	308	590	269	317	599	326	285	358	277
310	276	264	254	263	242	266	424	395	358	262
213	672	309	275	180	264	321	302	305	721	267
312	233	232	228	310	328	227	330	248	277	257
296	209	301	261	320	242	744	257	244	228	275
243	239	523	257	203	303	191	264	279	287	223
230	263	226	323	242	208	245	283	236	285	260
290	229	234	173	246	176	237	740	536	294	293
279	224	225	234	334	301	220	274	232	273	268
288	237	139	245	298	302	250	755	285	419	203
271	292	292	191	281	532	178	241	299	263	204
278	484	239	243	243	244	226	245	273	311	268
231	252	221	249	271	234	281	234	248	285	300
207	183	276	270	286	284	229	234	187	192	244
143	133	171	242	189	74	296	214	258	176	284
299	290	118	764	321	350	346	230	144	396	177
670	217	282	208	257	334	180	316	399	355	313
271	560	333	398	284	242	410	425	276	31	331
282	322	235	192	409	194	197	407	312	288	182
258	0	287	232	347	316	311	367	287	248	7
179	119	352	375	331	299	214	313	332	250	303
225	219	351	240	245	647	268	447	198	272	298
677	266	299	176	243	271	521	224	260	183	337
162	231	261	295	637	104	216	220	204	65	237
12	188	197	188	552	230	238	168	251	310	324
196	271	701	285	251	325	403	275	999	301	201
266	222	747	269	242	413	645	500	450	310	332
190	257	412	265	240	241	244	232	226	232	315
264	223	257	244	243	277	342	286	211	222	272
240	289	120	246	222	205	296	229	304	292	221
273	303	280	309	309	341	219	325	351	209	

528

2087.4_1313EC75	313	320	112	338	334	284	305	231	532	220
296	380	323	321	394	403	266	276	336	427	580
442	195	408	255	267	425	322	314	491	418	492
497	516	391	446	586	116	538	322	372	333	337
284	298	556	504	177	403	396	241	316	320	423
392	504	493	498	288	341	495	323	620	286	391
307	639	452	401	264	357	286	413	326	344	304
274	641	243	460	290	479	185	372	472	527	495
495	449	511	365	498	144	697	753	672	589	490
595	699	697	110	628	121	665	262	324	640	637
281	662	661	669	345	419	290	428	284	433	534
409	353	247	604	599	372	259	220	357	398	504
289	353	275	323	297	192	102	320	341	339	169
295	184	371	435	391	381	395	426	393	454	405
459	478	376	696	704	394	638	445	610	649	593
370	122	270	626	640	633	237	371	92	333	377
303	331	307	354	103	202	275	362	461	94	362
399	407	145	237	278	305	551	243	143	384	65
303	355	453	234	325	372	561	353	384	322	261
302	18	291	405	284	391	301	313	363	144	428
256	641	179	237	312	1	288	233	520	493	267
324	0	391	227	398	312	378	308	696	522	0
208	121	366	322	255	574	197	381	452	679	512
337	384	325	263	361	232	376	28	483	323	442
188	464	536	418	643	271	228	369	143	22	609
252	702	553	282	223	272	515	570	480	65	573
173	657	20	665	251	438	716	266	722	354	614
719	627	232	954	304	269	193	289	301	999	558
442	176	289	635	693	583	335	472	491	291	276
204	291	502	497	723	484	317	369	447	377	452
499	443	484	472	445	444	424	524	300	422	446
475	460	174	611	510	118	673	47	679	656	703
292	414	274	289	273	294	197	305	225	294	

529

2091.2_1313EC11	256	244	43	298	280	214	305	287	487	229
243	206	233	316	440	435	253	340	460	330	328
349	217	397	209	210	415	290	293	350	308	349
348	351	416	525	640	7	603	285	275	221	310
220	348	489	237	110	346	265	231	215	310	533
276	598	593	592	245	286	585	342	636	240	384
296	590	395	410	246	384	248	382	290	379	267
376	424	202	474	353	491	189	328	538	526	545
550	526	564	235	559	209	556	575	594	686	517
681	571	531	116	576	193	580	210	261	717	725
295	578	586	640	271	484	147	462	256	470	541
470	274	266	617	574	482	204	241	292	402	952
276	268	299	299	231	114	141	277	233	233	177
257	151	408	468	420	413	414	450	421	469	464
627	544	417	594	596	387	557	565	569	550	553
396	110	250	564	511	526	233	441	312	466	465
416	424	446	492	82	362	341	496	490	137	319
383	360	84	149	191	305	505	263	75	251	174
270	458	404	205	431	355	348	419	371	319	120
309	124	218	278	224	398	258	229	404	180	522
164	629	184	225	276	6	226	221	494	280	137
528	2	457	278	283	250	306	316	511	598	0
117	239	313	390	176	612	189	435	423	630	498
252	363	285	240	316	203	396	70	593	258	564
84	439	558	437	587	308	131	474	211	223	625
202	670	453	228	121	246	627	397	595	204	460
383	511	42	511	219	428	611	191	621	314	627
643	640	197	576	331	154	127	263	201	558	999
373	159	319	564	528	527	248	512	492	225	173
213	265	472	449	562	499	258	419	537	448	453
472	545	629	505	463	474	391	621	355	472	445
549	480	158	378	627	186	491	11	550	539	685
304	453	245	255	291	282	212	308	209	245	

530

2109.7_1313EC75	244	217	61	362	332	215	295	431	309	207
276	330	264	276	302	371	317	288	120	294	288
419	200	338	255	225	369	254	339	350	352	338
346	352	339	351	448	58	430	305	313	312	316
252	282	355	312	60	346	330	255	327	313	357
326	453	470	469	318	241	466	500	485	526	399
506	437	374	403	547	559	286	386	298	548	314
589	280	270	331	299	419	180	355	353	408	457
458	420	447	252	450	155	459	399	471	467	405
472	465	454	91	457	189	454	278	258	447	446
264	397	396	437	357	353	176	328	210	351	312
341	270	235	372	371	310	237	292	297	344	373
239	259	273	268	316	179	93	238	271	303	167
277	199	577	761	605	577	568	640	583	580	579
592	395	362	403	418	388	413	354	411	401	418
386	133	293	371	429	417	278	294	18	320	305
319	97	285	313	144	258	265	358	338	56	372
328	345	108	156	182	295	327	394	161	399	143
166	263	209	143	138	201	161	296	431	288	203
204	64	272	323	322	321	275	371	131	8	354
296	439	62	193	309	2	238	220	331	287	154
273	0	320	234	298	285	343	532	212	479	2
118	278	287	291	295	455	67	459	329	476	534
149	79	218	240	262	209	577	63	471	281	369
232	434	486	338	351	550	250	315	74	6	461
158	318	471	294	207	94	478	271	455	118	446
3	374	2	370	252	323	409	130	423	395	537
383	387	264	447	469	277	79	309	266	442	373
999	783	204	369	396	451	268	425	471	308	280
224	290	432	342	359	837	366	604	409	623	389
524	547	423	414	400	616	340	447	198	282	689
348	719	574	270	371	5	354	2	434	429	332
525	579	246	265	280	237	170	190	174	226	



531

2113.2_1313EC36	27	25	0	25	102	24	189	401	93	131
73	21	213	54	123	192	222	59	138	215	213
195	51	52	28	20	137	36	26	183	185	185
184	189	164	203	239	0	117	36	179	154	114
73	37	205	225	2	241	137	69	158	31	76
137	201	243	246	160	27	244	458	243	463	190
442	246	52	188	460	454	23	201	193	521	144
580	252	20	141	179	314	6	308	222	307	338
342	263	256	153	337	196	214	134	225	179	242
179	224	332	1	335	4	239	169	58	163	163
75	195	196	219	139	75	5	190	121	191	136
72	10	101	154	125	95	3	136	46	223	128
184	120	92	172	30	4	0	143	137	141	40
130	4	564	848	598	563	574	631	556	485	586
667	198	194	128	122	308	163	155	205	247	189
174	0	19	98	172	186	159	262	163	225	258
316	169	187	246	0	248	168	363	212	0	164
47	207	205	1	17	189	95	386	217	38	6
295	219	225	150	69	21	20	63	46	42	1
27	0	16	34	10	149	26	139	254	3	94
9	161	0	20	169	2	74	13	103	188	3
100	0	85	85	35	34	152	381	211	268	0
93	220	38	292	174	247	0	224	251	242	482
20	174	217	5	93	13	572	0	331	33	126
6	282	301	269	59	591	2	197	208	5	240
19	208	231	82	10	252	282	74	321	0	138
0	193	0	198	35	277	204	137	208	138	262
191	125	23	187	485	13	2	30	222	176	159
783	999	124	185	227	295	206	123	178	29	9
10	21	228	285	146	874	261	572	170	618	245
568	568	149	227	272	608	58	122	159	212	717
110	687	611	159	96	0	246	0	106	209	83
535	582	21	100	110	37	11	67	12	40	

532

2125.3_1313EC75	283	231	2	286	310	315	337	158	330	267
252	285	751	350	355	380	350	244	361	335	312
327	153	314	584	253	300	585	308	353	304	328
360	368	325	313	344	1	288	380	356	352	238
262	662	422	152	159	330	301	190	338	810	354
264	318	285	298	315	256	294	297	335	225	279
282	387	306	284	240	234	784	301	280	189	301
203	279	522	298	270	331	101	344	331	326	316
314	313	325	334	312	122	301	253	330	366	311
366	324	319	49	333	165	324	743	553	359	356
242	298	299	325	300	304	153	289	200	291	342
295	180	172	384	381	287	183	749	322	350	303
234	228	249	204	222	415	41	202	229	222	107
190	391	243	247	243	253	248	269	290	321	270
247	277	252	321	320	260	335	276	322	331	348
277	53	226	316	303	271	181	283	199	255	331
218	283	266	284	1	253	213	280	327	37	313
315	366	81	750	189	337	317	62	226	273	82
759	397	349	267	189	269	227	287	294	286	123
227	523	261	326	212	350	335	324	292	163	342
184	413	41	185	318	272	254	528	373	217	154
279	0	306	175	279	313	275	325	333	340	0
92	93	320	364	327	267	132	278	381	366	330
199	321	381	190	239	614	221	438	258	242	422
654	295	343	256	309	199	436	315	224	144	336
193	296	334	88	624	286	321	111	300	66	372
6	285	180	286	508	351	322	242	325	296	317
294	443	745	295	244	131	317	111	747	289	319
204	124	999	288	310	502	639	631	511	163	125
185	109	457	189	331	255	157	255	289	255	372
283	258	289	336	277	290	241	311	217	256	306
320	270	15	296	320	199	277	121	327	310	319
201	310	143	104	63	146	117	184	146	200	

533

2128.7_1274EC17	294	305	227	332	316	285	364	265	565	292
315	314	301	355	369	380	334	373	359	377	332
416	262	397	270	266	428	345	334	504	391	474
498	495	421	494	588	283	605	322	363	284	399
327	337	545	300	189	381	343	249	387	309	412
301	529	545	547	316	308	528	341	661	260	384
316	691	448	388	259	344	303	426	416	324	346
337	421	295	489	375	454	240	469	452	538	556
555	516	553	294	562	181	778	558	797	608	500
606	780	798	305	787	175	766	261	305	646	628
316	857	841	743	329	413	245	511	307	515	697
432	346	273	705	672	389	287	243	308	409	537
321	337	278	305	328	267	297	279	334	256	291
315	252	388	460	427	414	407	440	428	484	426
464	512	371	646	649	420	581	480	595	585	585
436	345	303	591	528	530	238	339	219	344	356
309	305	361	345	359	284	416	358	488	352	332
390	394	201	243	280	364	581	233	253	328	203
254	323	500	266	408	349	320	349	407	224	301
273	248	271	331	296	358	317	311	348	163	452
239	615	187	235	287	60	301	257	470	255	224
407	116	394	254	351	316	300	308	540	572	134
342	225	350	364	266	625	221	377	518	706	486
431	297	269	390	419	275	332	213	493	329	532
183	494	596	368	488	257	252	287	289	299	605
334	533	672	305	250	295	581	344	579	168	680
209	782	174	820	276	403	847	253	826	323	578
527	703	294	654	326	340	296	378	269	635	564
369	185	288	999	889	718	362	491	596	385	337
202	367	563	536	539	482	276	365	467	396	523
366	411	508	529	532	445	490	540	287	447	464
466	404	171	470	539	176	460	232	524	515	552
331	401	374	462	342	400	293	424	363	316	

534

2134.7_1274EC17	260	256	128	330	294	258	318	262	602	215
236	305	297	293	365	395	294	302	358	332	346
372	177	401	265	224	371	287	304	552	346	530
538	546	394	457	641	218	587	311	327	267	334
257	308	542	310	193	312	268	198	285	264	402
286	561	590	594	243	278	558	294	701	243	397
286	721	460	405	230	305	246	461	389	329	303
316	380	221	483	302	424	174	442	450	551	614
621	541	572	287	576	103	847	556	858	597	520
597	846	861	86	827	104	826	197	275	612	594
272	893	877	758	279	360	251	494	227	500	619
413	335	236	696	658	352	234	191	277	379	508
244	298	253	260	261	216	76	276	277	228	175
247	181	394	473	423	413	426	437	436	439	392
454	523	379	640	642	397	597	470	645	615	622
412	126	331	603	523	546	193	327	105	343	333
334	284	303	345	100	170	323	343	486	115	321
339	386	60	185	259	318	617	257	196	311	66
284	392	490	202	321	375	327	364	383	217	223
284	172	237	314	257	348	252	266	343	171	452
179	653	178	252	272	3	263	221	487	292	218
359	0	391	231	304	264	290	297	587	604	22
302	186	318	383	280	618	216	406	498	730	460
375	315	283	238	422	226	329	123	481	304	524
200	492	572	378	472	235	191	315	225	285	568
255	531	644	300	186	344	613	347	616	104	707
150	865	98	888	236	358	870	225	840	316	564
507	680	222	698	260	281	239	301	242	693	528
396	227	310	889	999	692	416	478	567	322	312
167	307	512	537	530	507	291	384	444	431	534
393	389	448	509	478	497	434	518	311	440	424
484	407	212	441	539	111	506	122	515	519	537
308	426	253	338	247	329	197	344	242	292	

535

2155.6_1313EC75	376	389	29	411	394	345	370	266	676	315
342	380	423	434	407	467	319	295	426	390	406
441	224	488	414	275	450	473	354	596	434	597
595	616	431	435	747	2	663	454	383	329	339
305	448	618	340	227	381	360	226	341	412	450
356	597	621	620	295	347	604	348	725	236	408
310	754	454	418	260	369	435	452	443	371	311
297	457	445	381	322	419	161	453	563	586	626
627	567	633	336	633	124	672	638	667	673	560
655	654	666	117	672	134	682	302	412	635	634
320	745	747	744	330	360	247	497	237	494	554
367	324	214	658	614	345	198	314	339	439	476
260	394	292	280	330	342	74	311	288	284	145
270	309	386	485	402	370	401	434	419	476	383
397	513	385	589	601	383	555	438	635	585	655
432	85	272	585	512	538	237	382	232	315	396
345	355	301	362	114	192	333	342	484	79	422
459	458	188	301	320	370	712	244	206	443	227
389	437	493	229	384	315	393	493	428	223	327
333	218	325	460	301	427	360	420	377	159	440
203	750	36	270	343	36	313	362	573	346	239
491	194	472	284	414	327	396	474	655	623	0
237	69	394	492	373	702	214	438	662	777	534
372	382	286	302	448	386	359	275	556	305	594
259	529	649	413	513	326	315	386	180	217	600
331	625	604	305	383	250	652	369	631	78	650
34	653	154	671	377	469	776	200	800	360	667
566	694	378	590	284	287	296	283	413	583	527
451	295	502	718	692	999	531	644	873	322	274
215	283	661	506	573	505	254	381	489	433	734
383	373	571	607	572	473	505	525	350	522	482
481	474	269	430	517	106	508	179	518	564	579
357	456	325	343	325	407	207	376	296	343	

536

2162.3_1313EC75	209	265	157	294	323	318	270	151	396	260
235	188	519	270	160	207	288	164	2	309	285
344	186	250	490	186	169	486	285	342	382	351
329	329	229	233	451	122	389	429	332	295	232
240	491	302	176	212	231	280	223	274	591	229
274	403	383	406	300	241	401	265	453	187	291
245	466	321	298	209	158	576	311	146	141	213
139	244	395	171	116	211	147	306	230	372	428
431	388	405	121	427	94	342	341	317	390	379
390	311	369	108	390	205	347	599	451	361	360
148	405	411	462	267	267	169	176	157	175	230
259	173	191	348	324	224	201	587	323	356	248
180	252	184	188	207	431	113	205	228	216	137
219	428	184	279	193	195	207	257	267	230	221
190	260	242	350	364	261	332	239	391	355	381
260	95	228	346	297	334	175	288	129	216	288
264	199	208	267	111	170	176	241	283	117	297
200	154	153	671	294	270	424	153	186	237	16
552	162	215	145	148	284	184	225	287	176	238
155	552	244	258	334	177	325	371	47	1	267
267	437	243	123	240	18	269	360	300	251	138
141	0	173	158	252	274	256	262	404	420	0
249	72	271	243	284	381	134	303	394	476	276
340	9	195	168	192	495	147	464	259	207	354
631	254	367	41	286	12	397	107	139	18	330
38	345	413	253	506	0	405	257	410	56	459
10	397	1	405	406	15	433	62	442	218	388
298	395	558	352	120	189	297	252	645	335	248
268	206	639	362	416	531	999	553	541	217	301
47	243	545	293	371	306	200	109	368	191	428
92	196	301	352	331	290	264	339	254	214	252
294	217	111	235	290	115	320	103	319	352	318
201	232	165	222	143	188	185	216	207	218	

537

2168.9_1313EC75	354	315	25	378	359	374	350	232	471	317
331	289	557	420	438	543	355	299	493	360	327
385	233	385	464	293	424	513	361	448	360	445
439	432	350	501	529	5	516	365	356	313	361
352	574	508	278	227	380	406	218	346	551	432
341	468	463	469	363	355	462	346	532	230	393
326	552	390	390	263	318	543	378	378	371	317
293	397	450	393	340	435	144	404	469	445	458
479	443	487	308	484	128	491	478	506	537	458
521	498	512	32	540	221	526	440	465	518	512
269	525	529	539	301	342	234	432	196	446	429
362	291	201	519	461	389	133	437	353	408	457
218	273	297	259	324	316	32	273	348	297	149
209	342	326	372	317	323	320	382	379	424	324
364	448	376	432	456	386	477	446	441	469	483
414	6	213	458	441	432	190	383	205	369	390
389	413	362	358	4	233	289	349	415	4	353
433	487	5	463	316	350	474	147	184	346	174
546	468	384	245	361	345	282	391	347	235	182
332	397	304	398	250	463	415	350	386	198	485
272	587	89	236	344	10	353	377	452	370	184
462	0	416	295	342	307	315	342	469	511	316
120	139	387	406	326	577	193	397	508	578	484
278	387	426	264	304	482	393	286	489	311	467
433	450	798	545	465	303	344	460	126	127	509
254	557	455	230	394	281	496	258	448	60	437
317	440	0	482	395	411	521	217	558	355	530
508	531	472	453	255	273	291	230	500	472	512
425	123	631	491	478	644	553	999	613	259	210
193	226	594	436	468	407	281	329	453	350	538
368	342	454	487	426	380	412	506	255	452	407
472	358	115	302	475	177	421	96	457	488	449
273	382	238	235	239	285	220	297	258	357	

538

2180.5_1313EC75	337	382	144	412	422	364	417	292	619	376
356	375	448	423	405	459	386	297	431	438	343
457	244	471	470	317	469	455	365	554	478	588
536	553	382	478	733	233	641	511	403	344	327
312	450	541	355	237	411	327	223	379	463	442
347	632	637	642	348	352	641	392	682	305	408
384	687	440	415	320	399	465	433	404	368	354
313	369	427	371	337	390	181	450	528	573	634
646	586	655	323	677	146	560	586	556	634	583
620	542	567	154	586	207	582	367	433	628	624
305	601	603	654	338	380	266	445	253	451	439
388	319	224	574	524	368	268	358	397	461	484
297	400	268	284	344	379	105	322	303	281	223
301	372	357	472	378	352	374	423	385	450	371
417	481	395	541	532	386	539	411	573	537	566
433	128	269	534	473	475	229	477	252	386	476
411	389	361	478	178	268	360	378	456	187	412
431	457	169	373	340	417	642	286	311	423	102
397	430	472	255	378	366	330	431	463	217	375
341	312	352	419	329	413	355	441	348	173	474
284	693	141	306	367	55	304	423	508	364	211
399	0	436	324	424	316	362	437	565	652	3
339	153	397	411	375	710	369	439	584	718	538
358	389	308	369	414	451	396	331	587	358	582
367	563	616	422	433	302	329	376	176	168	579
303	544	547	298	391	308	654	281	659	44	582
3	561	10	554	396	459	625	228	648	346	663
485	580	430	509	318	306	293	308	450	491	492
471	178	511	596	567	873	541	613	999	402	367
247	299	706	484	495	535	272	351	557	400	753
325	363	561	561	546	484	513	556	269	541	400
471	418	195	429	508	162	488	183	513	543	482
302	440	367	398	405	451	222	409	361	377	



539

2217.8_1274EC17	287	352	233	310	331	273	277	231	313	211
297	382	219	274	259	292	252	276	227	336	202
366	379	398	272	278	322	232	271	319	310	269
314	291	272	248	289	286	332	310	264	272	271
255	237	314	239	181	367	320	303	344	240	240
283	324	300	292	271	274	294	314	280	249	356
291	291	396	363	231	353	264	378	335	303	339
258	292	280	275	284	405	323	280	285	384	270
322	286	265	146	295	333	327	317	329	317	303
333	309	296	267	342	301	317	273	278	354	351
261	271	268	267	299	246	241	330	284	326	267
233	253	283	272	244	226	294	217	310	364	241
323	333	308	301	299	307	295	195	343	262	368
324	276	312	377	332	350	319	388	362	424	342
292	276	239	327	322	375	314	251	321	345	347
330	292	587	298	304	301	277	248	143	230	279
215	16	248	218	291	255	466	309	318	315	281
262	280	340	204	270	277	309	183	187	370	179
162	215	261	127	256	190	209	342	351	188	320
183	148	271	320	233	302	289	339	180	121	229
266	286	145	113	253	14	214	236	298	230	185
203	147	274	189	296	246	254	270	279	306	79
272	142	282	195	242	341	214	363	309	313	416
222	168	234	324	249	270	231	191	288	321	193
164	425	308	207	313	203	228	221	239	172	395
348	253	315	564	249	205	282	234	249	222	354
0	212	163	278	243	258	288	255	303	233	370
251	309	236	289	185	816	225	578	310	291	225
308	29	163	385	322	322	217	259	402	999	887
277	590	317	278	282	331	217	245	182	269	325
226	223	363	360	399	291	516	324	156	282	293
237	348	124	216	300	46	255	302	289	264	257
279	241	492	498	546	449	408	484	466	417	

540

2225.2_1313EC36	301	304	269	351	335	269	300	193	278	239
315	314	246	310	234	253	285	250	204	338	256
384	350	389	257	254	314	277	267	335	338	284
328	289	268	223	254	277	297	314	316	277	298
295	271	224	245	134	339	304	265	350	288	227
312	341	307	325	290	283	326	295	263	238	390
286	261	400	399	198	335	280	412	315	268	306
218	224	288	253	225	362	269	327	256	354	284
336	265	278	149	302	303	350	251	357	293	290
303	358	315	300	367	257	351	299	299	309	312
233	232	229	230	322	276	282	303	250	295	259
303	261	282	255	247	207	291	249	282	379	216
325	318	298	287	293	312	301	199	350	303	353
298	298	309	337	330	334	321	367	343	375	347
265	261	287	332	320	318	328	241	306	337	306
305	284	569	257	309	286	285	195	125	209	251
119	3	218	235	276	202	380	263	272	298	312
264	247	291	207	253	300	286	162	195	328	235
125	201	225	118	152	192	168	324	337	89	389
197	184	253	311	274	317	311	379	92	17	224
312	243	203	128	260	26	261	269	237	210	170
179	2	276	211	320	280	266	250	236	315	105
219	117	274	143	273	280	173	360	212	266	355
202	96	176	372	179	296	112	165	245	306	185
163	374	338	80	259	89	267	178	273	144	404
284	33	293	548	255	124	302	180	262	88	329
0	205	97	225	252	138	215	229	241	247	367
228	293	262	279	123	747	240	569	332	276	173
280	9	125	337	312	274	301	210	367	887	999
277	576	370	198	275	326	150	216	213	217	286
158	163	321	355	404	255	441	277	10	197	271
181	295	12	236	271	39	189	253	306	253	215
227	201	415	479	471	348	249	364	355	423	

541

2225.6_1178EC20	230	227	14	305	288	281	184	107	226	183
122	304	208	157	184	182	195	191	128	271	234
394	253	300	250	145	225	194	281	176	352	197
199	199	266	262	185	0	203	234	299	325	221
191	159	227	256	91	333	248	189	207	251	208
253	209	210	229	317	346	226	181	190	87	222
170	199	230	228	171	190	220	219	153	215	313
176	164	216	157	220	240	184	117	184	261	247
237	230	237	311	219	144	217	236	201	210	243
214	211	209	151	196	198	210	213	236	247	248
308	165	166	181	255	189	211	187	261	182	210
192	711	232	214	188	172	255	162	174	272	214
294	300	149	251	365	271	1	324	826	853	65
258	231	201	167	193	224	159	194	163	221	198
210	190	182	187	185	162	183	173	203	191	205
151	0	244	176	210	206	213	209	159	188	195
169	218	171	198	102	188	294	231	185	0	344
281	208	73	97	276	184	238	145	149	281	35
114	179	150	160	176	259	202	251	436	179	171
197	104	299	226	341	201	245	224	199	54	219
249	189	67	211	314	59	197	232	197	288	125
242	0	177	197	239	255	265	274	266	223	227
180	0	359	188	186	232	178	233	204	203	157
170	256	211	167	167	204	201	86	243	304	230
117	217	183	206	194	178	186	209	130	87	344
196	175	192	287	212	5	253	254	223	78	178
24	185	7	196	255	220	195	126	208	288	246
226	216	234	198	127	278	150	267	190	204	213
224	10	185	202	167	215	47	193	247	277	277
999	269	284	256	324	181	229	203	212	151	204
164	185	245	264	249	247	295	225	115	223	196
159	221	3	158	218	51	227	100	216	224	227
171	164	200	224	221	282	284	261	283	186	

542

2245.5_1313EC75	250	225	212	300	290	330	250	220	300	170
273	389	208	237	242	282	240	278	219	275	235
357	381	382	288	229	302	192	228	324	242	234
303	290	267	267	278	257	305	322	276	228	266
243	203	249	220	142	261	238	267	292	246	230
247	305	282	304	255	306	295	320	300	282	434
299	342	431	438	275	350	222	441	335	322	287
269	257	258	316	241	369	243	313	338	332	294
328	331	281	102	278	222	356	350	360	313	310
334	345	339	263	363	218	360	254	241	352	344
231	323	316	301	258	242	264	359	246	355	240
250	284	305	318	299	227	232	236	246	379	314
249	271	269	272	227	274	265	166	352	279	268
236	271	306	358	349	340	310	374	321	341	338
313	325	277	330	327	340	350	314	318	353	314
306	251	770	331	329	324	305	270	148	235	314
171	14	273	251	260	212	382	321	343	299	278
262	249	245	169	322	250	285	192	185	380	172
105	183	248	175	267	187	162	387	336	223	321
144	150	284	316	193	264	277	322	179	5	225
239	316	166	41	252	14	223	186	228	223	183
213	0	312	178	282	193	216	188	249	286	55
251	214	331	131	243	300	201	283	266	332	376
204	63	143	264	186	241	252	105	302	281	195
124	309	327	202	280	234	248	258	200	130	338
275	185	327	752	219	202	293	218	247	59	347
0	231	149	299	213	223	321	193	327	182	344
296	318	188	293	183	606	168	803	257	291	265
290	21	109	367	307	283	243	226	299	590	576
269	999	327	216	249	336	196	268	186	279	303
267	271	302	280	301	302	471	355	10	222	284
264	311	137	196	338	89	268	208	306	277	272
281	269	426	485	441	416	377	440	414	410	

543

2257.2_1160EC23	308	306	204	421	416	322	359	242	574	326
364	315	422	440	406	456	352	332	377	371	374
422	252	445	484	320	439	426	324	533	498	508
532	526	400	456	708	230	655	534	372	349	274
277	458	503	315	200	404	423	265	325	416	439
345	626	640	637	298	383	629	370	680	275	414
350	666	417	422	312	325	390	444	375	310	327
310	386	437	333	326	391	183	394	385	607	597
637	610	627	348	680	144	521	560	523	602	613
588	491	487	242	507	199	512	328	408	585	585
257	535	541	652	361	395	257	387	252	389	437
371	359	187	511	502	360	215	315	344	455	472
277	353	287	223	329	436	237	293	348	355	202
271	417	353	443	367	362	360	407	406	423	324
412	466	354	482	492	368	485	413	598	486	591
380	236	292	474	464	471	230	399	237	362	401
374	326	378	362	253	277	352	353	414	249	433
415	405	115	343	303	359	609	227	294	349	291
378	447	480	288	373	329	331	460	429	213	333
336	316	315	449	380	408	399	464	372	165	487
222	636	180	366	349	62	266	479	457	349	239
400	0	351	311	429	354	338	383	589	671	12
334	88	460	415	414	667	255	460	538	708	487
350	393	296	364	368	422	335	327	557	329	574
312	517	578	423	420	292	384	342	233	258	625
273	524	472	277	434	253	675	296	707	35	528
22	456	74	494	358	376	599	167	625	359	615
487	544	383	521	294	314	349	332	412	502	472
432	228	457	563	512	661	545	594	706	317	370
284	327	999	422	470	474	241	318	536	359	672
334	353	511	563	543	474	499	517	306	530	386
465	390	247	406	477	184	460	156	489	495	466
299	415	356	372	316	374	216	360	294	356	

544

2278.6_1274EC17	348	238	63	320	299	237	255	226	516	228
320	284	264	322	423	430	275	350	378	360	331
427	235	361	243	281	360	352	306	462	368	452
464	456	404	472	562	168	528	299	290	272	284
282	306	494	294	208	353	386	307	271	208	408
315	443	450	445	337	301	444	326	556	292	358
268	566	443	355	282	372	266	403	366	352	323
336	432	276	370	353	448	238	343	370	569	476
469	528	456	325	451	199	516	499	502	517	536
513	478	479	91	493	172	494	235	237	553	546
280	550	548	539	332	300	183	433	289	429	481
311	283	227	536	504	351	223	257	329	383	426
247	236	241	231	297	240	149	335	292	310	159
256	234	275	407	308	313	293	371	370	449	334
423	391	358	463	460	344	419	363	472	437	486
332	148	103	454	401	409	224	299	199	303	297
305	201	303	295	123	156	366	310	354	120	331
387	418	243	169	242	255	533	232	219	322	162
286	410	475	252	364	313	326	397	383	263	280
286	199	255	322	274	390	262	288	412	168	448
169	576	189	241	290	62	273	204	522	303	226
384	1	385	220	323	317	320	332	562	484	104
231	124	341	389	314	503	165	403	505	600	404
402	288	342	227	407	266	335	181	418	293	531
195	495	458	324	421	306	201	357	279	134	538
288	466	467	200	184	176	504	398	485	128	462
21	478	153	517	218	377	583	195	596	359	508
437	531	241	517	288	268	302	192	265	497	449
342	285	189	536	537	506	293	436	484	278	198
256	216	422	999	439	389	221	272	424	334	491
329	356	413	496	516	394	395	457	298	453	348
359	371	193	417	423	31	419	258	418	411	421
315	351	339	303	245	371	281	373	354	305	

545

2294.6_1274EC17	300	252	0	305	311	255	261	258	555	190
287	340	264	296	369	359	243	302	323	345	520
427	201	424	234	255	432	311	244	459	369	437
454	459	370	387	671	0	613	334	337	280	319
247	325	509	284	234	356	337	240	243	330	425
346	515	514	514	264	331	502	296	612	269	425
305	657	461	436	249	349	280	462	307	361	296
330	643	203	441	337	465	204	343	474	524	552
545	515	550	332	551	141	559	752	578	650	509
654	560	569	96	585	123	569	238	295	687	689
347	574	580	608	308	460	296	411	309	408	495
438	291	305	538	561	433	240	269	307	337	522
343	267	283	342	261	117	86	232	374	364	190
286	133	395	439	401	401	411	443	428	451	448
435	526	404	689	720	425	646	547	673	627	671
428	0	283	673	644	653	281	359	162	332	383
269	370	326	368	0	248	278	390	543	0	328
322	363	92	166	254	261	569	256	107	311	11
248	317	405	242	286	256	595	294	400	281	197
242	135	221	339	253	333	222	213	307	335	368
230	635	7	211	285	3	195	264	475	262	306
324	0	366	232	380	301	326	283	722	554	0
214	244	375	338	220	533	1	352	440	651	540
252	349	317	254	387	220	352	1	466	242	505
167	482	528	377	777	304	204	336	119	0	600
191	763	541	222	145	220	556	611	531	1	488
458	412	4	507	224	361	616	246	620	360	626
783	609	184	746	307	241	184	249	240	723	562
359	146	331	539	530	573	371	468	495	282	275
324	249	470	439	999	490	258	366	467	381	441
541	362	513	478	466	437	405	590	322	343	467
543	515	226	557	603	113	688	5	655	658	787
309	466	275	240	242	274	281	282	158	267	

546

2310.0_1191EC10	278	301	211	281	268	243	265	570	522	273
233	265	270	341	356	483	256	334	396	345	334
371	226	398	269	266	383	292	285	454	368	444
447	447	373	418	619	249	597	320	261	263	282
246	321	442	280	198	350	305	204	235	247	376
299	498	555	540	246	293	539	583	631	602	338
575	591	360	340	587	665	245	357	391	631	316
650	403	218	413	305	453	165	408	418	500	547
569	515	584	257	597	163	501	568	507	601	527
589	482	478	246	493	181	498	188	217	571	571
271	513	521	587	293	386	191	409	252	413	421
356	225	183	537	489	335	255	199	313	348	501
279	285	225	234	247	190	226	276	208	261	212
285	197	580	870	605	572	601	654	597	632	633
687	497	385	496	532	430	486	460	561	482	561
376	247	313	521	501	515	276	315	190	306	316
300	297	291	315	246	261	327	347	458	283	324
361	339	222	222	235	265	531	574	215	292	84
313	473	392	239	384	373	314	343	407	240	301
273	232	247	358	269	407	298	313	406	185	431
148	617	187	284	285	24	233	252	428	277	182
398	173	377	182	297	254	289	472	535	569	60
313	262	343	424	258	623	211	430	443	611	669
333	361	221	259	391	199	691	123	560	301	525
166	517	490	424	443	636	174	358	207	214	586
199	531	462	332	192	233	592	372	604	197	486
85	446	159	460	194	442	541	188	549	353	590
507	504	177	496	588	298	241	351	241	484	499
837	874	255	482	507	505	306	407	535	331	326
181	336	474	389	490	999	360	574	473	635	473
603	625	519	440	454	659	492	549	342	470	755
457	764	618	394	506	184	490	200	520	522	498
563	694	353	395	335	355	226	344	278	344	



547

2311.4_1274EC17	190	204	69	240	233	189	207	369	258	133
232	165	163	224	301	274	160	208	263	254	203
235	192	254	183	218	241	228	185	266	183	276
254	244	273	271	286	67	283	184	221	262	258
178	268	321	236	162	315	285	212	286	183	274
226	289	319	307	237	199	312	402	333	411	286
396	309	278	282	424	392	152	260	274	455	224
540	275	186	268	303	348	258	217	297	275	265
288	268	273	159	273	258	320	252	320	296	258
309	310	311	134	297	123	310	235	232	301	302
303	294	302	323	227	281	250	265	258	264	286
261	276	142	325	326	246	287	119	252	289	322
306	275	298	256	236	228	104	202	206	197	180
332	236	679	495	679	710	674	695	725	686	658
500	268	227	303	316	255	305	307	286	333	310
292	91	29	280	318	305	302	221	221	265	257
212	281	252	177	109	168	242	260	268	80	240
266	298	165	98	184	207	266	379	82	273	73
215	191	257	185	204	164	183	218	256	217	240
258	139	226	287	131	255	198	237	292	161	247
148	277	67	190	239	157	201	209	275	196	114
296	12	222	213	209	201	181	283	290	300	119
159	319	222	246	177	312	142	296	266	312	381
212	193	277	180	216	164	425	208	255	193	276
130	218	271	169	323	497	180	225	222	103	343
250	293	267	127	200	110	293	252	262	236	283
223	302	45	285	216	247	287	238	300	219	312
287	305	270	327	267	145	216	152	244	317	258
366	261	157	276	291	254	200	281	272	217	150
229	196	241	221	258	360	999	695	307	609	234
592	481	242	364	313	672	216	316	255	238	509
294	539	494	299	295	60	268	4	307	304	287
330	448	261	342	235	357	201	252	266	227	

548

2328.1_1313EC75	239	233	11	254	264	205	266	525	357	191
223	227	281	267	344	378	247	260	318	326	290
293	178	316	210	229	322	281	243	343	288	340
349	370	322	320	444	6	400	239	254	274	277
271	263	335	261	126	318	319	199	258	214	330
219	370	406	392	273	230	388	508	451	530	317
499	422	310	309	561	548	232	282	294	608	289
752	344	199	381	282	384	130	326	340	340	368
372	339	389	231	381	183	440	409	433	431	355
455	429	430	76	408	139	425	232	244	455	456
249	437	439	448	253	344	152	286	187	272	312
301	260	159	378	393	257	219	225	283	324	422
229	237	219	207	232	202	62	223	240	291	134
221	243	971	665	961	965	946	924	914	742	853
722	391	293	428	446	297	407	375	380	387	385
245	66	222	431	442	441	287	264	116	272	267
301	286	264	279	114	232	310	308	354	7	270
338	359	161	207	190	266	368	529	154	233	70
287	349	301	183	297	349	227	305	341	235	222
316	169	317	357	197	345	263	248	339	134	363
217	455	159	233	267	1	275	211	347	258	94
316	183	351	221	269	215	228	368	409	419	43
163	276	269	330	203	408	239	379	320	439	508
236	353	329	196	256	148	640	124	430	299	396
179	321	399	388	389	676	148	329	167	274	431
203	429	432	252	163	271	414	288	381	2	365
86	430	138	406	223	424	443	155	444	287	466
392	390	161	385	465	235	247	231	232	369	419
604	572	255	365	384	381	109	329	351	245	216
203	268	318	272	366	574	695	999	413	919	350
813	655	378	304	309	906	359	432	264	358	655
358	773	755	331	395	231	423	96	447	452	396
462	642	299	321	307	394	240	339	328	226	

549

2339.5_1160EC23	195	188	123	325	303	197	287	209	435	263
262	221	206	325	349	345	289	375	312	274	278
324	167	305	226	242	375	288	291	308	358	329
300	304	344	403	629	120	586	340	280	225	306
205	299	464	281	116	283	249	215	231	274	421
285	609	599	593	233	250	584	288	648	269	360
275	607	402	366	248	307	241	385	265	449	264
427	317	187	383	259	372	194	328	392	510	637
631	543	613	219	613	208	491	486	508	688	531
672	486	482	128	504	146	489	203	215	627	628
249	487	495	607	320	444	169	320	244	333	470
418	187	218	540	521	419	199	214	283	331	515
232	241	269	265	187	145	132	275	222	260	129
253	187	410	436	421	408	411	453	398	431	432
428	547	494	526	523	453	503	492	533	483	526
438	142	255	486	486	478	207	332	191	348	335
381	335	322	311	117	303	330	330	478	180	351
295	295	84	175	171	287	474	214	186	228	182
271	347	306	189	344	288	254	401	363	306	149
296	174	162	253	294	301	210	246	278	150	407
134	652	190	215	266	15	219	209	438	305	137
438	71	413	274	268	238	321	277	437	662	83
164	174	291	384	236	581	241	442	481	643	457
215	340	375	253	357	197	402	74	677	250	590
106	449	533	475	430	318	184	325	198	126	571
229	512	449	237	136	294	629	379	610	140	468
254	380	67	416	225	360	534	216	552	359	617
460	558	159	480	236	143	173	202	226	447	537
409	170	289	467	444	489	368	453	557	182	213
212	186	536	424	467	473	307	413	999	410	476
437	332	655	520	491	466	359	577	423	488	465
501	449	251	291	516	190	455	142	511	484	466
287	420	268	287	275	293	210	280	219	238	

550

2347.2_1313EC43	268	266	81	246	276	233	242	536	421	153
205	195	276	295	329	362	217	285	320	297	239
242	226	329	235	176	335	280	199	364	326	353
361	375	340	320	473	176	428	256	214	253	248
276	269	371	232	192	330	305	229	227	242	344
232	382	422	408	264	232	406	532	464	532	305
531	492	346	299	534	592	261	289	340	641	257
740	320	205	401	332	415	202	339	337	365	436
443	395	448	214	451	135	485	427	482	452	404
477	473	466	107	463	196	470	211	221	453	454
253	457	461	480	190	352	215	319	242	307	357
297	219	177	391	385	284	244	200	276	366	430
272	256	173	205	209	221	99	231	280	274	142
248	229	904	703	922	894	931	934	894	742	837
700	436	327	437	460	318	409	387	430	373	451
296	86	269	396	451	449	250	277	192	274	281
309	321	270	296	113	263	354	298	373	67	296
343	384	209	230	230	242	441	562	146	207	143
270	370	338	208	338	278	158	302	321	278	258
272	135	264	353	209	330	248	251	380	6	354
240	537	205	216	241	80	280	211	370	218	144
369	214	361	206	281	235	238	341	427	452	1
256	269	267	296	205	434	204	350	336	464	561
248	362	310	238	311	191	680	174	395	256	448
182	365	451	333	382	682	198	349	261	160	457
183	447	457	282	194	228	450	291	426	76	423
220	460	145	430	243	423	465	131	471	256	463
416	435	182	380	517	262	201	271	232	377	448
623	618	255	396	431	433	191	350	400	269	217
151	279	359	334	381	635	609	919	410	999	363
761	658	438	342	350	905	425	428	266	378	669
374	790	739	329	409	167	417	275	462	459	406
465	645	315	344	352	436	300	375	359	318	

2383.7_1313EC75	358	292	84	318	354	295	473	278	675	494
402	373	355	436	429	512	460	336	425	377	269
395	204	519	348	280	498	361	257	584	378	628
603	596	429	476	621	0	560	442	385	276	364
346	346	582	272	185	413	397	179	349	319	458
260	569	580	580	282	369	574	361	550	322	550
332	621	545	556	302	322	323	543	376	334	314
331	345	350	400	334	413	146	389	413	589	597
603	619	613	294	622	141	617	503	640	563	595
565	621	624	2	632	193	646	265	350	560	560
271	529	530	555	287	430	259	495	213	498	490
442	283	194	593	517	348	109	278	376	355	384
229	303	332	264	296	195	23	212	308	251	177
193	215	351	390	367	351	355	392	356	393	363
363	446	374	492	493	361	499	394	537	474	565
420	1	352	463	462	428	208	372	193	349	378
339	337	322	385	1	184	292	365	405	1	338
394	452	154	184	289	473	656	266	387	424	264
293	452	468	239	360	327	308	488	375	201	347
396	99	353	462	219	479	322	385	438	288	503
261	720	152	258	337	1	331	364	586	270	174
437	0	423	320	392	258	313	390	613	628	0
150	160	391	477	401	594	179	356	676	589	479
223	451	325	242	470	260	365	13	478	289	591
155	605	616	293	413	306	220	379	3	21	552
318	511	588	322	243	311	589	155	554	1	545
0	514	0	541	248	414	551	277	597	297	593
407	622	280	433	316	295	127	299	315	452	453
389	245	372	523	534	734	428	538	753	325	286
204	303	672	491	441	473	234	350	476	363	999
368	373	434	618	598	454	435	467	272	500	377
425	397	103	401	455	1	365	62	478	508	400
249	387	252	243	232	280	204	263	195	296	

2386.9_1160EC23	248	211	2	237	310	193	313	463	404	291
253	237	305	231	353	338	304	265	340	364	377
310	162	300	232	192	400	331	246	348	294	320
371	357	314	330	470	60	439	256	318	278	268
305	259	381	294	129	347	365	160	270	231	341
242	327	362	364	288	265	356	418	435	410	312
400	459	313	321	423	490	241	305	299	574	296
676	531	232	397	231	427	147	369	375	373	404
404	401	416	286	423	129	421	571	410	476	387
478	407	420	11	415	150	411	240	263	515	515
233	409	412	425	209	340	215	326	212	327	331
344	255	121	390	398	356	122	242	236	317	440
213	187	251	242	283	89	94	227	271	276	182
196	164	800	642	797	811	795	812	782	710	847
719	417	284	479	525	292	446	436	506	463	480
294	138	336	517	490	515	212	304	135	290	312
303	328	274	266	12	219	276	333	424	114	291
346	352	32	233	188	313	412	445	163	249	10
306	398	330	181	347	307	457	288	302	246	88
243	3	221	256	149	374	218	255	353	218	346
231	504	61	310	337	2	302	267	376	272	227
324	0	331	234	292	270	247	377	506	387	0
56	243	269	324	203	340	136	334	338	449	551
287	364	334	228	278	152	599	1	364	289	379
80	322	436	300	563	590	170	355	145	219	457
234	601	331	215	172	270	400	432	308	61	340
470	372	2	394	214	462	420	212	430	305	453
575	459	160	504	456	200	114	224	264	499	472
524	568	283	366	393	383	92	368	325	226	158
164	267	334	329	541	603	592	813	437	761	368
999	648	397	324	340	821	332	470	191	345	685
443	779	670	417	492	134	523	6	511	510	590
458	718	213	192	208	306	168	268	150	217	

2427.1_1274EC17	222	216	109	254	284	207	276	494	402	204
243	210	272	278	367	384	275	317	374	276	257
225	153	326	218	291	322	271	214	315	253	364
328	331	285	410	402	151	356	220	270	256	306
229	297	303	238	155	321	319	169	221	263	317
231	317	356	355	275	221	354	509	363	455	263
471	357	308	267	486	535	255	291	338	554	218
606	314	178	372	311	426	193	337	354	360	360
344	419	343	273	376	147	397	378	397	380	404
381	396	399	131	350	239	360	196	206	445	444
240	395	399	393	240	312	215	314	240	315	365
341	224	185	379	365	299	270	208	249	305	506
275	261	249	223	236	118	147	275	237	248	202
267	172	658	662	653	666	664	677	675	687	713
931	334	332	397	417	326	376	399	378	382	357
313	178	243	371	378	383	277	344	265	316	344
288	303	300	358	186	234	296	327	339	189	302
294	292	111	153	192	276	394	491	141	243	13
291	369	297	234	381	329	330	287	271	262	208
259	123	227	246	173	387	244	205	348	199	397
195	428	205	196	280	58	262	187	340	273	159
381	1	350	275	189	258	251	375	412	358	0
240	280	207	300	186	386	198	287	326	388	456
221	357	293	193	301	203	571	226	379	226	316
213	318	361	321	415	566	126	299	179	163	461
254	450	305	270	176	284	349	232	268	180	319
284	394	106	426	247	376	422	216	418	276	341
434	420	232	414	547	220	146	265	223	443	545
547	568	258	411	389	373	196	342	363	223	163
185	271	353	356	362	625	481	655	332	658	373
648	999	378	315	320	679	404	419	252	327	702
394	657	632	379	412	206	368	208	380	373	462
532	658	296	317	328	374	263	325	265	282	

2474.9_1274EC17	221	235	203	313	290	256	263	246	468	251
252	264	245	361	354	370	258	432	380	333	294
386	265	388	246	232	366	293	315	337	386	334
329	318	445	407	599	245	620	376	328	263	356
264	319	439	277	199	346	296	199	327	283	417
307	564	557	551	279	353	553	333	608	271	349
289	589	370	355	259	432	252	375	370	335	302
385	326	246	419	246	441	187	393	462	524	583
590	551	586	226	597	198	488	522	509	711	528
716	493	509	310	552	210	518	232	281	686	694
274	480	492	595	318	387	200	440	279	429	466
410	250	269	525	487	390	231	212	313	471	575
284	268	264	314	253	207	284	313	281	298	251
262	196	410	470	434	407	430	475	432	445	469
483	643	566	596	615	545	574	566	596	576	583
549	273	276	576	542	551	236	353	186	403	363
367	349	364	384	295	320	371	402	592	312	331
340	344	107	172	237	263	486	235	125	283	136
240	345	366	259	465	288	331	387	397	301	241
248	199	241	302	322	395	400	334	376	196	402
219	604	247	251	263	24	285	228	404	296	169
462	0	478	285	384	246	328	315	442	599	165
243	195	390	377	288	654	203	465	444	609	577
266	276	223	328	394	267	342	147	698	318	511
180	511	625	442	503	239	262	342	206	195	566
365	555	488	284	221	259	587	397	566	137	547
224	427	172	412	271	426	546	207	548	375	720
514	527	212	510	400	307	178	320	257	484	629
423	149	289	508	448	571	301	454	561	363	321
245	302	511	413	513	519	242	378	655	438	434
397	378	999	480	435	455	439	698	457	533	443
623	492	201	360	632	119	537	196	590	564	579
458	470	378	404	362	382	229	409	319	350	



2493.1_1313EC75	296	304	94	357	331	272	340	251	600	309
301	320	341	393	367	396	313	334	347	392	312
403	222	423	316	273	396	362	340	471	440	501
470	464	332	395	639	101	606	420	313	333	301
422	347	450	295	209	476	403	272	297	314	381
292	536	549	553	282	331	549	324	618	286	384
304	623	409	389	321	323	329	417	370	360	395
298	379	332	429	289	470	218	457	450	555	579
564	518	588	321	573	141	520	487	512	584	524
584	509	477	62	489	183	499	227	389	553	543
346	540	552	604	299	332	272	408	289	406	430
337	299	213	508	491	339	320	241	270	408	474
348	332	234	251	333	280	58	305	290	266	170
357	337	331	434	350	351	340	384	350	508	325
370	459	372	501	498	348	488	432	592	493	602
362	51	276	525	439	438	205	402	317	366	401
399	374	351	393	112	248	366	379	415	99	375
408	410	174	249	264	340	621	247	240	338	251
322	410	450	253	377	343	319	418	416	175	307
287	236	297	358	305	369	296	321	329	214	410
237	638	129	318	309	105	448	343	485	307	182
437	141	415	340	378	330	324	341	518	585	119
373	146	360	403	359	601	332	428	508	634	402
353	396	344	287	362	347	365	306	490	385	541
201	489	519	384	436	292	270	400	320	163	587
316	504	560	270	324	243	623	265	647	153	554
232	484	157	518	365	395	572	196	618	345	557
462	538	318	497	269	345	356	312	244	472	505
414	227	336	529	509	607	352	487	561	360	355
264	280	563	496	478	440	364	304	520	342	618
324	315	480	999	924	433	466	532	306	488	411
454	415	273	388	511	180	437	195	471	485	455
299	402	392	449	363	481	309	427	398	380	

2518.0_1313EC75	301	344	252	362	351	259	356	274	563	329
321	289	261	419	380	383	336	335	363	372	332
402	248	421	298	283	394	307	276	454	406	473
470	451	308	371	632	311	644	419	316	307	336
440	347	440	265	207	461	430	259	328	316	369
278	512	527	530	271	320	525	329	605	307	360
314	617	393	365	314	365	324	397	357	368	420
339	394	321	387	269	437	205	445	436	543	527
532	503	545	288	521	165	482	490	478	581	519
587	472	452	279	483	206	479	204	411	562	543
273	506	519	561	274	318	260	412	244	413	434
337	301	201	484	493	317	244	164	281	407	455
291	334	268	241	306	294	262	262	311	270	215
286	337	344	423	365	358	349	388	370	487	336
375	411	367	492	483	333	457	384	537	463	578
355	252	286	480	432	428	205	315	261	330	331
331	352	299	350	284	218	401	342	396	274	361
381	384	189	199	249	356	589	269	275	322	256
248	374	459	223	378	311	317	414	406	211	321
283	251	271	352	288	362	341	317	304	192	379
219	629	124	323	305	53	441	332	453	254	189
406	132	390	382	371	335	271	315	514	552	203
365	142	342	351	340	590	352	426	482	639	440
322	382	275	352	358	307	375	226	485	419	523
164	509	466	388	425	316	242	369	267	212	573
343	498	501	291	309	226	583	309	605	107	508
179	452	144	475	366	398	538	234	586	297	559
458	564	287	472	288	371	337	317	243	445	463
400	272	277	532	478	572	331	426	546	399	404
249	301	543	516	466	454	313	309	491	350	598
340	320	435	924	999	409	484	485	264	472	432
408	427	253	386	455	164	418	214	474	474	459
342	392	398	450	356	463	313	415	371	363	

2564.4_1313EC75	287	268	2	304	286	280	299	517	460	250
257	234	340	311	323	373	260	281	273	344	322
330	208	347	296	249	362	338	309	411	308	413
389	399	354	387	518	1	472	351	311	307	276
268	329	387	297	168	298	267	267	257	287	343
281	474	503	501	271	285	501	565	520	528	319
564	514	358	318	536	545	286	344	336	656	295
746	345	277	424	349	396	254	418	335	431	458
477	467	472	275	485	198	475	510	480	513	466
514	499	505	66	506	150	511	249	288	493	496
333	516	520	518	261	343	244	360	260	359	393
347	288	209	439	433	324	340	245	291	384	452
292	309	256	232	304	291	53	306	246	249	183
345	276	908	730	916	903	932	945	917	812	875
755	452	328	442	478	397	435	417	514	403	470
388	1	290	481	461	474	241	278	188	270	282
346	304	303	304	40	260	342	340	409	2	336
331	343	140	238	260	299	482	522	201	266	171
320	368	365	229	287	342	302	351	386	288	293
254	189	267	307	243	298	282	338	375	118	401
234	565	202	262	290	218	282	296	394	296	166
345	1	379	240	298	278	324	389	489	498	46
243	263	320	317	297	490	262	400	397	521	581
333	313	328	264	358	288	692	201	440	309	462
238	411	491	362	400	660	277	335	249	225	540
176	466	490	312	265	268	500	359	486	176	529
23	458	166	444	316	396	521	215	524	300	503
464	484	253	467	454	258	243	297	277	444	474
616	608	290	445	497	473	290	380	484	291	255
247	302	474	394	437	659	672	906	466	905	454
821	679	455	433	409	999	467	468	330	463	682
402	801	760	391	444	176	444	253	467	472	440
441	680	372	413	366	501	280	399	384	255	

2578.1_1274EC11	392	382	213	392	370	345	343	313	528	303
355	421	363	378	444	465	307	350	408	421	352
480	328	486	362	335	466	376	340	484	429	439
482	456	436	414	456	266	472	404	400	346	380
326	349	416	303	214	445	423	337	438	382	404
373	428	404	403	378	346	404	439	429	358	421
396	496	458	431	356	498	345	455	453	452	416
375	415	340	406	424	530	291	433	459	498	438
461	485	436	320	463	245	474	502	478	495	462
500	464	494	261	513	270	507	357	357	521	513
378	422	420	407	381	373	327	498	343	495	375
385	329	360	424	413	382	356	319	399	401	385
354	325	330	377	397	301	293	305	387	329	405
408	253	394	459	440	441	414	484	482	500	449
430	443	411	450	454	463	446	378	460	440	447
424	265	366	407	437	445	338	424	192	397	415
372	213	376	367	274	322	516	449	372	274	361
365	350	300	212	337	343	538	302	196	457	181
268	378	391	204	324	301	279	403	470	274	338
267	112	363	472	347	429	353	355	382	140	402
322	499	125	143	359	13	317	342	384	313	246
357	0	386	249	358	326	367	331	420	459	63
235	222	401	312	323	480	177	430	374	490	544
254	252	296	349	351	306	453	89	384	372	384
154	535	527	206	337	358	268	372	224	66	496
375	338	431	447	283	231	453	227	393	116	487
0	383	210	403	312	423	425	224	457	345	503
406	508	338	409	315	493	215	485	342	424	391
340	58	241	490	434	505	264	412	513	516	441
295	471	499	395	405	492	216	359	359	425	435
332	404	439	466	484	467	999	448	166	339	459
332	438	82	350	416	124	331	347	434	406	385
345	318	412	438	379	432	393	494	439	460	

2619.2_1313EC75	252	292	52	320	292	264	263	253	524	235
263	325	250	311	324	374	241	380	281	338	315
429	265	445	231	228	398	265	289	367	396	371
364	345	401	461	661	13	601	367	332	274	324
251	293	452	285	169	357	299	253	279	266	469
321	572	560	578	268	324	557	347	665	278	421
323	642	429	436	279	442	246	448	329	376	339
350	392	250	457	242	474	198	410	481	511	608
609	564	607	258	611	156	546	559	553	723	551
721	540	547	80	557	187	531	214	278	699	677
306	548	561	628	307	463	248	475	274	477	498
452	268	308	578	544	436	242	237	331	454	558
287	292	277	337	324	160	99	277	305	292	253
288	163	411	469	437	444	426	511	448	486	462
477	892	460	786	794	487	822	825	762	790	745
474	71	341	833	795	780	274	410	172	435	435
369	367	400	414	68	338	355	472	822	86	328
363	299	219	178	250	263	555	273	105	314	152
214	324	355	198	397	304	353	404	426	309	212
263	132	254	326	315	331	338	267	320	267	445
254	610	186	216	313	4	261	226	428	307	213
433	0	399	259	359	257	348	350	511	600	150
241	185	369	357	282	632	193	428	462	677	530
277	268	277	251	378	214	326	159	636	344	533
136	522	614	407	580	200	234	416	205	170	611
315	631	556	286	175	227	617	456	585	147	541
345	464	89	497	231	471	607	188	602	351	824
604	574	200	558	383	281	143	334	286	524	621
447	122	311	540	518	525	339	506	556	324	277
225	355	517	457	590	549	316	432	577	428	467
470	419	698	532	485	468	448	999	396	433	477
878	601	206	617	836	164	729	141	822	826	678
394	600	374	389	379	338	230	391	289	320	

2651.1_1160EC15	124	144	165	110	189	118	151	56	219	121
129	116	102	135	254	168	107	332	181	189	104
149	44	171	158	122	209	122	139	176	156	192
180	176	241	330	307	0	265	203	152	159	315
212	238	334	136	8	306	253	201	218	199	294
224	307	280	293	171	187	276	252	333	134	181
221	306	255	191	98	307	94	216	263	181	185
279	205	17	272	275	336	188	264	264	379	338
333	306	320	129	322	141	257	259	265	411	293
405	278	317	19	321	161	309	266	228	398	398
133	270	275	299	249	243	75	279	200	293	273
267	117	184	339	299	258	67	152	203	278	315
137	147	210	231	160	70	99	149	218	163	182
103	7	262	329	274	278	263	307	277	322	267
321	349	508	322	339	721	302	286	330	328	325
481	0	144	299	283	281	199	307	138	263	320
277	187	255	284	1	205	244	305	310	0	220
141	291	2	3	36	151	205	12	38	123	13
98	183	143	114	312	101	140	130	188	253	8
106	0	124	104	94	159	142	107	218	2	299
6	362	17	133	151	0	224	199	289	91	64
290	0	264	205	144	242	234	208	263	312	68
31	214	208	273	128	309	3	222	263	338	321
102	135	107	139	278	122	135	117	407	218	358
49	289	398	266	283	173	79	216	43	3	306
107	333	284	10	108	21	318	276	352	16	304
23	305	2	247	134	230	301	85	311	145	401
318	316	180	299	177	128	89	10	211	300	355
198	159	217	287	311	350	254	255	269	156	10
115	10	306	298	322	342	255	264	423	266	272
191	252	457	306	264	330	166	396	999	249	327
320	316	153	200	336	6	324	0	311	306	339
322	286	96	145	9	94	8	113	11	81	

2656.9_1313EC75	305	279	224	295	312	292	307	206	402	238
319	283	325	325	400	417	285	362	418	355	273
329	246	294	266	268	406	293	273	388	326	378
392	375	425	408	543	266	559	343	350	248	335
303	311	524	295	114	445	313	230	315	292	469
286	502	492	492	300	267	491	335	498	245	374
308	538	381	378	248	370	280	384	399	335	300
313	339	261	391	356	466	188	375	441	515	524
530	507	536	279	536	159	458	452	471	532	491
533	462	512	215	554	178	532	250	275	525	524
286	455	450	483	300	397	216	472	255	477	510
413	310	254	556	518	401	135	182	395	379	434
237	269	295	291	243	143	227	275	330	226	221
215	171	358	425	411	395	397	467	439	450	448
442	480	447	445	425	429	426	412	457	478	481
448	263	166	418	397	405	241	352	88	349	377
350	336	347	375	222	259	319	362	429	247	322
338	385	288	156	252	307	389	92	192	329	206
303	383	464	278	359	289	251	361	305	155	211
298	126	291	314	130	384	286	236	405	204	365
212	526	21	242	313	79	290	228	423	322	209
399	3	364	330	258	196	277	322	453	537	47
243	281	297	351	275	467	107	365	472	516	509
247	429	343	367	315	224	335	99	496	272	529
100	466	534	406	362	271	77	387	167	229	457
383	465	411	197	184	306	516	242	455	2	323
0	370	0	411	213	445	469	252	479	328	534
421	536	207	410	321	244	192	229	222	422	472
282	212	256	447	440	522	214	452	541	282	197
223	222	530	453	343	470	238	358	488	378	500
345	327	533	488	472	463	339	433	249	999	411
420	418	118	325	409	9	381	74	397	437	399
388	396	266	268	250	273	107	248	177	199	

2679.2_1160EC23	223	216	163	288	258	240	278	511	393	256
257	233	258	316	315	414	231	304	342	361	246
315	243	355	224	244	337	279	252	365	260	360
351	340	328	389	472	201	471	289	227	241	392
273	277	387	237	211	379	328	200	298	236	364
236	410	400	406	202	303	398	522	460	527	310
484	436	341	315	554	569	274	326	396	628	320
604	377	251	392	243	507	173	381	440	434	409
414	369	408	200	421	146	411	426	400	479	378
479	390	394	199	401	196	404	206	298	491	488
242	436	436	462	244	333	175	357	230	364	422
353	224	158	407	388	379	209	231	236	368	427
273	294	256	273	257	212	207	217	235	265	177
253	186	615	721	633	624	621	701	655	710	726
731	423	384	444	456	342	426	426	461	439	449
390	226	297	451	414	421	256	366	220	317	369
288	322	297	292	203	248	350	322	431	248	288
346	330	101	243	227	278	423	499	148	270	188
254	404	327	239	379	317	305	378	366	304	249
250	215	247	296	192	306	280	245	340	169	380
162	467	176	271	240	19	279	274	343	253	157
453	1	396	234	286	260	257	465	445	432	95
225	209	328	404	267	483	201	322	384	471	524
272	349	241	282	375	187	668	175	407	285	392
147	444	514	346	453	601	218	408	224	214	512
220	537	394	263	221	239	437	318	405	90	414
300	386	138	413	284	406	441	148	478	287	480
495	459	218	453	539	258	207	294	272	446	445
689	717	306	464	424	482	252	407	400	293	271
196	284	386	348	467	755	509	655	465	669	377
685	702	443	411	432	682	459	477	327	411	999
463	712	619	374	462	154	453	155	431	455	491
618	703	344	390	372	380	203	391	340	354	



2687.5_1274EC17	257	316	56	292	276	211	268	224	422	259
270	269	261	307	309	355	248	313	290	313	286
362	180	382	203	218	350	249	238	307	329	311
317	291	362	423	585	0	523	316	287	235	266
274	311	423	267	174	330	267	184	255	288	467
282	506	489	498	263	298	475	310	568	233	405
266	544	392	413	224	400	243	413	312	318	285
311	397	279	400	246	425	151	355	479	471	521
519	506	497	258	519	183	470	518	475	625	496
626	461	468	43	469	151	455	213	276	622	619
295	513	528	549	260	434	226	390	241	399	417
420	266	289	467	452	421	190	250	291	413	500
241	250	271	316	278	124	79	252	287	264	141
260	164	354	399	377	388	362	431	395	468	426
443	887	389	786	780	435	826	964	739	830	716
415	40	286	842	821	834	207	411	158	402	414
398	419	388	393	41	325	265	426	886	76	323
290	289	148	175	194	268	423	203	59	262	190
238	359	338	138	326	307	333	327	354	258	124
265	2	235	273	222	334	323	214	325	198	409
226	573	187	259	289	3	292	241	407	305	229
408	1	349	295	344	224	310	374	467	503	0
93	190	321	322	255	563	162	345	399	578	492
176	356	287	261	324	229	331	141	562	282	483
129	449	540	353	590	233	208	332	189	83	567
279	635	471	183	176	211	527	387	504	110	424
382	409	2	459	212	441	527	202	527	318	747
598	474	178	511	375	216	159	226	240	475	549
348	110	320	466	484	481	294	472	471	237	181
159	264	465	359	543	457	294	358	501	374	425
443	394	623	454	408	402	332	878	320	420	463
999	574	174	647	936	93	747	92	828	842	682
366	576	287	290	283	251	116	299	207	241	

2718.4_1313EC43	248	265	106	280	257	246	283	521	397	225
262	269	265	298	306	379	229	318	266	295	315
353	239	364	261	268	342	302	281	359	301	350
358	341	333	363	488	150	483	304	249	260	295
249	322	380	250	203	309	271	251	266	267	354
271	419	462	454	236	256	445	543	489	541	366
528	451	363	369	558	589	238	373	303	617	284
692	410	232	402	303	393	220	406	404	379	453
446	346	452	200	465	179	448	488	451	490	371
489	431	423	199	425	230	419	247	257	477	480
261	399	403	458	261	356	255	351	289	359	354
335	216	213	380	380	317	328	248	244	387	472
304	300	277	292	247	244	176	285	243	237	140
330	252	766	765	747	746	770	785	756	698	774
745	533	326	543	555	385	526	557	532	517	499
351	167	244	553	561	564	217	324	237	307	323
365	311	328	306	238	326	377	356	509	208	308
337	340	169	231	231	283	429	531	116	274	212
283	368	317	259	366	264	371	350	375	234	280
259	258	288	337	243	315	322	329	359	166	370
183	472	224	254	260	115	264	260	329	247	164
386	98	359	269	293	235	288	445	433	457	173
294	279	301	272	321	486	315	402	389	510	607
294	263	307	263	373	277	658	277	456	297	394
224	440	426	331	552	599	246	289	317	175	513
307	605	448	253	224	283	478	456	470	227	444
373	377	185	421	261	373	437	190	464	324	551
598	439	249	441	522	328	258	277	289	460	480
719	687	270	404	407	474	217	358	418	348	295
221	311	390	371	515	764	539	773	449	790	397
779	657	492	415	427	801	438	601	316	418	712
574	999	756	467	585	169	561	264	577	567	554
539	743	427	466	397	465	334	424	405	337	

2723.7_1160EC23	1	95	0	125	168	55	134	436	118	57
197	127	62	132	204	171	146	169	1	169	72
89	7	113	71	112	180	84	62	83	90	62
94	86	189	165	204	0	190	163	120	122	164
109	145	213	109	19	231	116	105	190	115	195
76	171	201	195	102	101	190	471	202	486	207
487	206	162	209	497	399	111	178	134	508	152
647	222	144	207	210	244	86	249	193	221	246
243	237	243	5	268	50	243	163	236	210	248
242	244	216	5	220	78	182	149	71	199	189
175	195	195	205	95	198	218	167	201	178	183
204	254	190	173	158	149	140	97	112	253	142
188	198	200	200	160	86	4	45	244	88	60
156	34	754	742	768	765	768	777	739	635	746
654	209	192	203	226	244	219	178	219	221	217
229	4	9	203	258	199	216	219	84	227	214
264	114	173	261	5	232	189	307	197	0	64
116	163	166	11	2	134	88	429	57	139	321
60	197	5	0	5	78	18	12	84	79	106
1	5	72	73	54	75	98	212	0	0	138
98	244	0	1	123	2	126	90	186	11	30
168	177	141	218	164	38	76	392	167	173	0
122	328	96	7	153	171	116	179	179	219	336
115	2	236	28	262	142	530	73	203	126	234
15	249	271	198	105	545	138	168	122	5	249
69	202	188	61	18	160	244	217	247	1	261
0	181	136	173	141	211	216	123	237	111	253
201	155	176	197	417	105	77	125	120	174	158
574	611	15	171	212	269	111	115	195	124	12
3	137	247	193	226	618	494	755	251	739	103
670	632	201	273	253	760	82	206	153	118	619
174	756	999	121	184	0	252	177	236	189	184
476	585	177	185	144	217	3	94	140	101	

2733.0_1313EC75	330	303	49	248	285	291	306	251	518	220
289	376	335	289	363	456	277	271	368	373	461
357	150	361	266	271	401	334	262	519	313	484
559	537	347	380	522	73	468	325	338	294	252
274	298	391	313	223	314	321	230	271	251	436
344	458	437	439	240	285	435	293	420	262	433
281	469	468	432	239	320	238	453	371	302	264
259	554	262	404	267	412	161	325	463	442	380
381	463	394	340	383	123	511	533	517	441	459
469	519	487	118	488	99	499	233	251	524	524
304	502	514	481	276	429	216	469	227	451	398
412	286	214	394	427	334	200	210	307	375	360
257	316	255	280	287	206	101	283	293	280	130
263	178	355	340	358	362	367	410	385	402	352
390	674	278	774	751	330	840	642	667	808	639
291	120	264	720	825	819	199	360	183	356	364
354	303	326	364	106	176	264	365	676	129	270
360	385	161	183	256	306	541	210	194	359	22
307	372	391	228	291	308	481	330	343	260	252
351	227	345	405	235	403	319	259	348	139	396
161	539	205	218	348	0	261	228	412	307	287
350	0	342	228	358	258	360	278	605	420	2
186	82	341	341	264	397	172	239	420	486	421
290	351	285	248	374	270	304	119	352	250	428
158	407	374	240	491	252	214	343	216	86	463
353	513	451	218	197	278	407	319	377	49	370
116	466	151	535	219	444	532	293	541	297	586
497	460	231	569	344	245	212	209	246	611	378
270	159	296	470	441	430	235	302	429	216	236
158	196	406	417	557	394	299	331	291	329	401
417	379	360	388	386	391	350	617	200	325	374
647	467	121	999	610	97	762	3	820	821	590
267	494	237	258	192	254	174	273	189	264	

2748.2_1274EC17	258	295	176	302	281	251	282	237	500	251
244	311	257	290	318	383	260	367	303	330	312
402	251	447	240	256	383	276	264	370	352	359
371	351	404	475	629	221	552	324	315	242	322
226	287	456	268	172	365	304	243	296	248	511
313	533	528	536	261	313	520	322	615	271	404
307	602	396	429	255	427	234	435	333	353	306
315	430	263	448	278	460	214	402	507	493	571
565	513	550	242	553	233	526	560	521	655	499
651	516	515	205	525	215	502	233	271	666	665
337	591	604	610	301	461	257	451	282	454	513
452	275	333	543	541	471	293	264	314	432	577
312	336	272	347	296	174	220	249	280	281	238
335	182	388	446	416	415	403	477	428	469	436
481	862	428	774	774	470	792	949	748	804	728
455	246	310	809	782	796	239	404	245	420	399
383	446	401	397	247	374	352	476	859	277	316
358	324	183	211	244	282	536	246	149	295	129
218	329	425	229	411	299	357	383	396	296	243
254	185	248	288	252	320	322	274	342	273	447
209	586	186	216	276	103	240	206	418	287	214
439	3	394	227	343	249	351	311	490	540	102
258	183	341	356	259	584	208	355	442	625	538
303	262	228	274	372	210	342	220	572	324	533
158	469	586	348	633	202	231	392	270	174	590
299	664	523	271	185	225	582	418	546	218	496
402	442	160	518	249	445	615	204	614	336	753
647	540	217	557	361	284	212	324	222	510	627
371	96	320	539	539	517	290	475	508	300	271
218	338	477	423	603	506	295	395	516	409	455
492	412	632	511	455	444	416	836	336	409	462
936	585	184	610	999	183	740	215	801	800	722
364	574	363	405	349	363	255	413	317	316	

2770.4_1160EC15	131	214	0	118	150	99	145	74	142	2
251	146	231	97	152	189	131	137	38	277	160
121	89	82	189	56	110	182	183	124	188	43
127	80	168	200	139	0	137	172	210	216	247
227	167	77	104	59	189	185	154	177	195	196
125	150	180	182	94	149	168	143	176	156	90
190	185	104	86	162	187	185	75	150	94	209
134	157	211	159	161	214	161	183	203	147	139
88	101	140	208	92	215	148	136	151	181	100
175	157	130	5	149	136	128	263	182	162	173
135	189	181	183	158	152	220	175	142	145	125
126	179	176	196	193	213	181	237	167	217	227
153	121	194	156	188	190	102	207	191	125	100
173	134	191	194	208	225	209	231	232	217	180
181	177	198	114	122	180	115	157	169	169	153
194	103	128	180	111	103	175	161	0	188	185
136	3	191	148	97	90	141	219	163	123	165
72	221	155	140	90	145	126	91	0	164	1
231	231	156	3	3	181	88	123	107	0	39
43	163	28	102	175	141	103	143	56	0	203
163	95	92	82	181	175	81	213	37	168	77
89	0	94	197	128	44	119	89	116	202	0
107	82	127	1	56	78	179	152	5	95	164
49	0	69	110	34	187	91	152	165	201	5
124	143	167	6	117	144	232	209	77	2	129
161	0	132	50	206	172	72	41	85	25	123
0	3	130	2	185	103	132	1	166	174	132
133	75	221	129	19	65	76	77	205	118	186
5	0	199	176	111	106	115	177	162	46	39
51	89	184	31	113	184	60	231	190	167	1
134	206	119	180	164	176	124	164	6	9	154
93	169	0	97	183	999	12	142	127	8	162
308	83	96	112	127	61	0	148	164	95	

2811.2_1160EC39	292	275	0	330	317	251	261	264	512	245
269	336	305	269	303	385	252	272	234	344	455
382	179	386	239	180	392	346	284	463	379	415
469	451	361	350	602	0	528	337	343	298	262
257	328	455	316	180	386	383	214	283	324	389
380	526	495	504	259	319	501	332	591	268	449
289	600	486	455	238	401	250	474	308	312	268
305	538	249	424	285	484	162	369	479	477	475
476	482	482	288	477	113	576	686	583	594	481
594	586	593	203	596	94	599	268	285	602	602
309	532	537	547	337	446	242	396	247	409	452
431	312	267	482	497	388	206	278	326	386	487
259	271	262	297	286	165	187	315	332	337	161
267	162	422	431	440	454	429	486	453	484	438
431	735	372	837	842	432	864	724	734	860	710
376	161	240	810	895	888	271	377	157	331	368
316	304	324	327	161	239	270	385	756	0	358
232	369	192	143	259	261	528	255	164	342	13
237	386	340	212	218	281	486	321	317	236	197
271	4	281	403	246	318	276	304	353	324	344
248	604	205	201	289	1	240	243	422	297	285
359	0	349	200	365	265	363	331	617	521	0
141	168	348	303	248	518	8	316	447	617	529
228	393	301	205	362	240	326	74	441	170	450
202	467	516	371	652	230	222	359	122	3	545
214	679	516	259	161	205	505	553	489	1	477
209	473	0	542	222	439	561	199	568	351	707
691	534	230	676	319	204	154	247	296	673	491
354	246	277	460	506	508	320	421	488	255	189
227	268	460	419	688	490	268	423	455	417	365
523	368	537	437	418	444	331	729	324	381	453
747	561	252	762	740	12	999	0	890	884	744
283	523	259	188	110	276	186	262	136	212	

2826.4_1313EC75.144	278	82	216	271	111	159	139	84	76	
242	57	96	155	130	190	141	149	98	261	40
215	173	149	138	237	209	155	213	152	201	109
203	192	212	147	101	177	154	66	211	198	200
109	114	234	156	88	242	213	221	260	84	165
227	244	196	208	256	135	210	230	155	207	167
212	176	236	166	204	300	110	184	279	149	135
169	247	161	248	213	305	194	133	244	253	229
208	226	220	5	261	259	180	184	188	226	219
228	184	209	147	221	229	241	255	120	262	266
169	126	129	142	223	164	66	245	245	247	102
131	121	216	176	158	166	205	233	260	244	194
241	159	186	241	211	98	209	105	252	4	269
244	77	203	291	274	286	275	288	225	278	275
236	214	162	188	182	271	205	192	172	255	178
211	237	74	207	219	190	318	178	186	193	205
14	0	211	107	177	65	403	257	260	218	165
39	190	287	91	8	159	7	196	23	11	0
134	192	175	0	5	134	4	136	169	6	126
2	65	2	161	68	236	115	161	201	0	48
96	232	0	0	224	0	7	76	82	203	99
44	0	222	0	98	166	28	185	179	240	2
225	126	173	10	58	139	120	174	125	107	277
76	1	154	140	140	52	88	102	58	41	0
78	311	7	0	105	11	55	58	123	0	165
306	1	16	107	75	199	214	79	91	16	240
0	1	167	3	50	135	66	48	80	103	116
3	50	150	212	9	304	133	178	229	47	11
2	0	121	232	122	179	103	96	183	302	253
100	208	156	258	5	200	4	96	142	275	62
6	208	196	195	214	253	347	141	0	74	155
92	264	177	3	215	142	0	999	179	6	194
306	97	257	277	158	319	267	378	423	110	



2871.8_1313EC75	295	295	86	320	318	282	302	243	510	292
286	338	305	313	343	414	276	351	290	369	417
415	251	423	267	264	437	364	318	481	387	438
503	479	404	414	650	77	574	358	378	299	327
269	331	476	303	229	361	349	232	305	310	456
339	580	558	572	290	364	551	326	619	262	513
300	636	507	526	268	377	297	526	335	328	306
314	492	284	464	271	459	181	374	488	467	541
542	500	532	264	543	149	604	651	605	630	490
642	599	584	108	591	154	579	242	299	649	649
329	568	585	620	305	487	256	426	269	436	486
464	332	244	540	539	410	251	237	323	446	518
295	330	247	287	320	199	111	315	323	326	193
293	216	435	457	448	453	441	498	464	476	450
459	835	423	884	869	446	925	818	777	897	718
398	83	302	865	978	964	217	395	189	358	385
366	391	349	367	88	277	342	396	830	95	327
404	358	174	200	271	302	542	211	197	342	153
280	385	372	219	404	321	443	397	407	283	262
342	187	351	395	296	357	356	318	358	207	425
249	626	204	235	340	20	277	249	447	296	283
398	0	385	258	378	280	366	373	576	590	37
221	143	415	398	320	585	196	373	486	656	554
285	320	268	218	393	252	338	142	522	289	500
214	484	558	353	636	268	264	382	225	126	609
302	690	538	270	196	238	563	498	528	99	499
432	514	132	564	262	489	620	172	621	323	773
658	570	231	683	389	258	213	308	304	679	550
434	106	327	524	515	518	319	457	513	289	306
216	306	489	418	655	520	307	447	511	462	478
511	380	590	471	474	467	434	822	311	397	431
828	577	236	820	801	127	890	179	999	968	711
361	566	332	365	322	361	199	378	298	292	

2906.7_1313EC75	272	295	1	319	320	273	291	271	545	244
262	327	319	277	353	393	276	332	362	372	419
411	187	413	240	239	389	368	302	501	400	472
524	499	364	399	648	0	571	330	364	326	297
294	286	474	310	203	366	352	208	328	328	432
350	586	557	573	307	314	553	337	629	244	501
303	635	514	512	259	386	292	525	361	306	298
300	522	290	446	265	494	161	397	480	489	539
543	516	533	290	552	129	591	663	588	631	501
642	583	607	58	603	120	601	230	294	659	660
331	562	575	605	323	480	267	432	251	440	486
450	307	230	552	560	398	240	218	342	398	496
285	275	227	281	313	147	56	301	332	306	172
285	150	437	451	445	455	446	494	471	456	455
466	828	395	880	870	434	925	819	779	910	736
404	3	274	868	964	986	211	371	169	353	383
367	389	353	359	30	268	284	385	828	2	353
355	362	179	216	273	291	559	253	155	334	18
310	405	379	218	326	340	437	329	393	281	241
333	70	301	393	288	366	340	293	347	169	405
233	625	183	261	321	1	300	262	443	315	262
427	0	399	248	357	277	374	376	622	576	0
220	158	360	372	249	581	99	373	485	674	550
282	363	354	231	365	242	338	74	495	271	505
186	464	576	395	617	261	239	418	153	8	580
324	683	539	230	201	302	558	507	529	45	505
329	480	1	551	234	494	612	223	613	330	760
659	591	216	656	383	225	140	270	292	656	539
429	209	310	515	519	564	352	488	543	264	253
224	277	495	411	658	522	304	452	484	459	508
510	373	564	485	474	472	406	826	306	437	455
842	567	189	821	800	8	884	6	968	999	711
368	581	274	288	229	262	157	276	193	296	

2929.8_1274EC17	239	286	42	279	272	217	273	237	533	236
248	337	254	273	294	362	233	321	323	368	500
404	228	408	217	209	435	284	245	413	361	398
412	401	357	407	658	4	595	302	328	284	327
234	319	455	300	219	339	336	219	269	303	469
341	504	472	486	257	323	469	269	601	239	382
282	598	394	393	255	369	240	403	247	323	271
299	650	220	453	262	417	184	344	493	505	512
524	497	553	296	527	150	581	747	590	680	489
680	583	596	40	597	194	586	212	277	687	688
310	565	584	629	263	432	231	445	275	448	495
412	277	294	550	572	401	211	232	299	352	667
285	297	227	329	297	117	72	263	319	295	155
258	148	422	450	426	430	439	474	435	433	438
533	580	426	758	782	398	704	656	727	722	704
407	67	277	753	689	694	241	384	159	375	392
381	482	339	383	39	322	293	421	635	68	304
341	352	113	195	213	273	562	232	79	300	143
239	369	416	170	378	339	599	348	379	286	184
260	154	219	315	266	324	298	219	324	226	386
217	623	181	243	300	4	248	230	436	277	272
421	0	370	276	349	303	327	317	657	555	140
199	195	343	297	226	554	169	334	440	680	522
301	330	251	199	372	186	337	108	535	283	473
120	454	548	355	832	243	212	305	178	171	587
261	846	503	260	145	228	551	581	527	108	472
633	466	97	542	220	445	633	166	642	290	684
856	587	188	733	373	204	100	282	221	703	685
332	83	319	552	537	579	318	449	482	257	215
227	272	466	421	787	498	287	396	466	406	400
590	462	579	455	459	440	385	678	339	399	491
682	554	184	590	722	162	744	194	711	711	999
361	509	290	274	339	308	207	334	248	266	

3081.9_1160EC23	212	244	186	214	214	233	237	422	308	253
231	200	228	271	234	317	205	283	281	280	217
289	239	263	239	245	281	239	198	260	253	238
279	257	269	285	310	210	367	257	214	248	386
254	290	249	163	152	322	254	184	257	233	247
196	249	266	252	280	317	266	464	318	487	232
445	310	253	237	485	529	248	242	371	478	255
499	288	261	266	245	384	199	258	351	332	229
229	263	260	176	257	247	269	347	258	380	276
386	257	254	256	263	221	261	221	268	391	394
227	293	299	317	190	213	164	323	231	314	275
210	192	151	292	278	214	240	209	248	375	294
255	271	258	224	218	183	257	191	253	167	211
269	216	440	571	447	457	451	487	516	538	498
511	371	373	349	365	392	338	326	349	370	349
363	247	242	332	336	344	242	223	116	285	277
247	269	296	255	278	189	400	231	377	277	230
322	324	258	214	231	237	330	439	183	221	147
233	307	262	241	337	293	207	354	297	198	265
226	185	234	254	181	322	367	255	266	163	301
151	315	243	225	248	110	271	258	285	185	150
280	122	307	224	302	257	230	427	267	282	109
251	268	291	280	257	406	210	294	294	332	459
255	310	190	318	288	249	507	202	326	262	278
134	363	319	214	266	480	225	238	292	206	352
409	299	302	222	208	248	300	288	268	220	337
30	278	161	311	289	369	310	175	306	253	381
287	289	261	317	678	272	186	272	273	292	304
525	535	201	331	308	357	201	273	302	279	227
171	281	299	315	309	563	330	462	287	465	249
458	532	458	299	342	441	345	394	322	388	618
366	539	476	267	364	308	283	306	361	368	361
999	565	385	401	378	397	251	397	386	269	

3183.2_1160EC23	235	232	45	297	281	210	277	358	377	295
229	234	224	242	304	365	263	297	304	293	265
286	140	302	217	267	329	258	267	354	293	338
334	318	324	339	502	3	461	273	255	224	288
223	276	409	214	135	345	270	156	304	210	374
237	407	413	416	245	259	407	431	445	387	361
404	447	361	368	400	495	236	366	328	494	237
571	357	229	364	256	428	140	356	401	396	420
441	411	453	238	461	92	417	456	407	536	421
562	402	426	61	414	106	406	236	220	532	526
236	413	423	462	241	374	184	403	206	412	400
364	240	145	365	371	346	176	238	240	341	415
217	228	288	237	278	105	104	196	267	255	128
234	109	641	698	619	640	648	669	664	669	697
700	603	364	555	564	361	571	550	535	575	513
371	109	282	577	534	541	233	343	92	340	339
293	293	313	302	60	231	289	354	548	129	319
310	373	106	174	199	277	401	353	37	265	62
217	380	335	161	357	286	320	310	298	281	167
279	37	252	265	232	323	297	250	360	308	341
214	481	188	249	258	3	249	241	376	258	168
322	0	332	276	281	220	250	469	440	432	0
122	201	266	326	255	455	97	330	382	476	506
198	362	263	205	305	183	519	67	445	235	414
126	432	430	332	415	486	174	356	134	143	462
282	478	384	259	176	256	465	368	436	17	367
33	359	73	401	232	408	459	161	448	311	579
450	449	176	418	500	208	73	249	303	414	453
579	582	310	401	426	456	232	382	440	241	201
164	269	415	351	466	694	448	642	420	645	387
718	658	470	402	392	680	318	600	286	396	703
576	743	585	494	574	83	523	97	566	581	509
565	999	294	283	300	331	149	307	216	252	

3270.3_1313EC36	241	343	184	300	314	267	249	323	260	238
320	244	236	292	309	266	261	314	294	345	209
287	337	266	229	344	315	250	253	296	286	232
290	265	278	240	272	193	298	309	229	307	257
273	256	245	211	221	455	304	320	349	253	255
290	304	275	268	289	302	275	470	258	387	299
444	266	356	311	372	446	271	315	383	347	355
335	341	306	381	321	548	314	313	370	367	279
293	290	266	175	284	279	314	335	315	358	274
354	302	299	309	313	293	317	298	298	377	377
299	264	268	254	274	298	265	357	344	366	283
307	300	289	287	282	256	310	252	334	388	278
356	328	340	324	338	270	281	230	348	249	422
343	304	396	397	411	451	402	481	461	536	399
378	324	262	352	348	395	376	309	352	435	338
389	312	244	304	365	363	363	327	140	338	338
257	78	345	245	373	289	482	372	404	351	308
252	336	355	168	242	249	281	334	196	251	159
177	207	209	112	271	223	207	324	284	284	285
187	164	264	324	239	333	347	385	237	110	258
236	290	202	100	230	180	242	230	200	147	201
270	129	342	229	332	263	256	328	218	289	92
329	227	293	220	299	297	261	291	226	279	451
260	137	257	386	229	291	298	173	280	331	172
180	437	352	109	249	237	287	373	280	240	354
368	207	295	316	253	226	276	218	204	127	368
148	265	186	237	281	315	263	247	260	237	375
250	304	293	307	299	480	242	410	280	274	245
246	21	143	374	253	325	165	238	367	492	415
200	426	356	339	275	353	261	299	268	315	252
213	296	378	392	398	372	412	374	96	266	344
287	427	177	237	363	96	259	257	332	274	290
385	294	999	674	698	551	364	549	468	336	

3301.9_1274EC11	242	337	239	316	307	236	270	311	279	228
334	249	231	275	327	314	256	350	275	358	255
315	404	302	227	343	324	247	250	337	293	266
317	302	320	288	283	287	340	300	273	271	327
290	274	259	238	192	492	343	290	373	269	262
268	389	358	364	286	312	362	510	319	417	340
487	348	383	345	387	521	279	348	428	384	408
359	347	314	389	324	552	318	354	399	425	338
357	346	342	174	344	306	388	345	396	394	329
403	392	387	356	417	279	409	323	302	432	429
288	316	310	315	286	351	268	380	353	383	365
366	308	334	355	326	276	287	264	311	441	299
371	361	379	337	342	310	334	246	363	268	417
342	293	423	484	457	494	442	530	530	576	453
400	371	333	404	409	434	420	340	401	465	398
416	350	329	352	410	403	375	356	207	349	388
250	110	369	291	389	300	555	419	444	372	292
284	315	324	125	230	270	257	306	181	264	203
142	261	255	112	234	238	111	239	306	197	307
159	108	243	319	265	357	354	378	187	153	281
246	292	175	130	228	102	270	252	216	172	240
257	50	348	250	334	285	256	331	200	348	86
304	232	311	108	326	331	274	319	203	335	471
253	74	261	386	213	269	304	211	270	382	225
166	465	373	127	249	233	288	318	266	221	406
334	48	388	389	245	218	347	251	294	141	422
1	354	200	276	276	273	314	232	317	248	422
258	311	298	339	285	521	258	509	309	289	255
265	100	104	462	338	343	222	235	398	498	479
224	485	372	303	240	395	342	321	287	344	243
192	317	401	449	450	413	438	389	145	268	390
290	466	185	258	405	112	188	277	365	288	274
401	283	674	999	567	480	328	522	428	437	

3337.9_1191EC10	195	299	82	311	312	185	253	258	241	190
297	219	226	268	297	283	257	298	247	322	184
294	336	292	188	299	265	196	225	259	243	207
250	201	304	260	265	123	280	265	244	259	274
263	237	270	215	176	396	325	276	345	236	279
285	296	272	266	271	256	275	434	280	342	330
396	292	370	335	332	437	272	343	389	313	373
311	319	301	360	336	512	269	286	375	359	296
320	310	298	177	294	245	281	331	290	371	294
390	278	281	198	306	298	302	286	282	406	414
324	276	277	277	307	284	272	381	321	372	255
303	327	331	323	299	255	323	238	304	384	303
331	338	339	340	334	253	209	159	343	268	367
331	273	355	394	391	392	380	445	422	475	419
379	361	265	352	345	380	337	324	323	374	329
394	195	319	319	345	344	354	327	162	344	358
224	14	366	267	237	299	474	422	369	205	283
233	289	334	86	168	253	226	268	145	228	128
101	183	164	44	182	197	1	274	325	293	286
100	79	199	302	239	276	332	399	221	205	254
243	283	179	71	206	64	222	221	188	206	198
236	81	362	213	326	246	244	304	166	305	38
266	165	235	27	301	307	279	322	131	262	418
333	16	213	319	183	240	302	169	295	342	217
101	413	359	105	265	229	264	355	197	196	357
332	22	276	395	223	216	265	219	158	153	386
0	238	171	181	243	368	297	170	235	238	372
237	269	262	309	250	493	156	439	309	273	291
280	110	63	342	247	325	143	239	405	546	471
221	441	316	245	242	335	235	307	275	352	232
208	328	362	363	356	366	379	379	9	250	372
283	397	144	192	349	127	110	158	322	229	339
378	300	698	567	999	536	400	527	485	368	



3350.3_1274EC11	273	379	129	298	326	275	280	306	351	239
326	307	271	314	355	330	269	320	264	367	263
328	309	357	243	301	345	272	278	358	320	321
371	330	332	319	322	167	333	330	311	295	315
277	301	249	272	239	457	331	351	343	303	327
315	364	337	330	326	300	335	500	293	382	358
454	337	387	362	388	453	300	361	412	367	365
400	316	310	359	384	530	338	366	378	422	366
361	389	381	222	363	231	372	389	368	385	369
386	366	351	160	363	315	373	301	298	406	410
340	308	309	295	322	333	233	409	383	417	279
344	333	332	337	309	291	311	274	374	396	284
367	356	314	366	348	248	188	249	355	301	361
349	243	471	466	503	525	492	570	575	622	466
447	336	290	359	363	378	365	331	379	413	388
392	164	248	317	362	364	347	341	170	330	370
259	134	351	298	177	245	544	393	385	140	284
321	400	330	110	244	280	322	252	148	316	159
181	277	238	119	291	239	138	312	345	234	295
180	132	274	333	240	372	301	381	277	236	308
259	334	152	113	301	36	250	277	248	227	259
294	0	371	260	330	279	315	374	262	359	22
261	177	305	193	319	346	255	318	293	299	464
329	199	301	331	277	262	306	158	288	331	214
142	472	358	163	229	292	280	316	218	190	419
317	216	364	318	228	170	357	228	309	103	382
0	275	172	232	267	340	292	217	305	299	383
278	308	330	317	316	437	183	407	341	294	282
237	37	146	400	329	407	188	285	451	449	348
282	416	374	371	274	355	357	394	293	436	280
306	374	382	481	463	501	432	338	94	273	380
251	465	217	254	363	61	276	319	361	262	308
397	331	551	480	536	999	447	571	521	312	

580

3358.2_1191EC08	246	305	152	237	290	190	211	265	244	158
294	228	214	252	276	287	212	214	223	300	188
275	242	305	104	352	290	213	274	281	256	167
261	259	233	216	254	214	238	196	238	283	228
207	193	233	178	188	335	265	327	269	232	265
322	285	222	214	298	189	222	352	221	327	231
335	235	315	233	320	361	234	253	355	347	265
290	348	219	284	359	398	288	220	382	320	239
255	247	219	214	247	289	244	243	270	285	260
277	253	259	162	272	296	290	331	241	314	322
284	251	253	254	307	201	251	358	348	358	170
209	335	328	165	207	200	288	295	359	285	242
321	277	233	335	275	148	213	177	328	320	321
332	114	312	331	321	351	337	362	328	389	305
365	213	205	248	237	291	235	199	244	298	252
265	210	153	251	239	236	342	357	159	304	368
210	161	347	285	102	137	510	348	316	167	215
120	291	306	193	168	211	218	260	144	150	117
168	175	152	186	108	219	8	260	216	199	145
104	0	207	279	176	317	151	222	241	4	222
166	245	51	155	220	5	195	210	226	115	182
196	0	288	200	135	137	248	209	146	247	0
275	85	175	52	192	156	78	251	211	236	337
204	170	309	189	239	166	194	2	206	200	183
4	379	181	315	241	170	147	217	181	6	203
323	219	248	291	140	63	225	174	173	152	245
0	194	249	172	154	295	259	200	201	171	255
248	221	210	236	99	413	118	353	219	197	212
170	11	117	293	197	207	185	220	222	408	249
284	377	216	281	281	226	201	240	210	300	204
168	263	229	309	313	280	393	230	8	107	203
116	334	3	174	255	0	186	267	199	157	207
251	149	364	328	400	447	999	434	413	203	

3380.0_1274EC11	235	351	135	260	267	261	263	291	334	225
297	275	253	258	327	302	245	312	250	366	264
304	288	330	238	328	351	259	265	373	301	307
357	321	350	339	347	173	335	328	276	288	303
254	273	287	235	219	453	320	310	331	269	339
309	381	354	343	310	309	345	457	330	367	359
418	355	391	362	361	470	289	370	426	355	352
334	373	298	364	382	497	303	345	403	454	371
375	388	358	213	373	253	395	395	397	420	363
430	392	386	174	391	346	392	334	309	453	467
362	334	335	325	323	350	246	441	397	445	294
362	299	342	367	332	313	341	300	376	422	330
382	327	288	376	333	275	189	235	324	281	418
355	248	389	425	415	437	402	470	439	515	396
384	349	281	407	409	406	398	360	388	439	398
373	194	284	359	394	404	383	341	146	380	371
238	109	353	338	226	274	596	423	414	196	254
306	358	327	134	219	263	328	277	153	275	142
167	248	252	224	241	236	178	306	325	254	265
196	141	252	337	203	327	319	351	280	161	334
237	400	199	155	254	121	219	257	277	165	223
317	5	373	248	308	246	280	345	302	358	44
264	213	309	175	296	386	247	324	249	348	479
325	140	260	310	278	274	318	186	289	336	255
162	471	378	203	307	260	288	317	300	200	421
336	250	389	377	240	240	338	246	291	153	418
212	333	199	295	270	314	325	223	333	289	420
307	348	294	342	326	489	213	426	325	305	308
190	67	184	424	344	376	216	297	409	484	364
261	440	360	373	282	344	252	339	280	375	263
268	325	409	427	415	399	494	391	113	248	391
299	424	94	273	413	148	262	378	378	276	334
397	307	549	522	527	571	434	999	685	354	

3401.9_1274EC11	230	342	47	235	258	228	240	281	285	195
276	267	241	216	282	261	230	262	207	362	273
279	306	278	249	281	289	243	244	321	267	204
300	222	266	279	265	151	248	326	251	281	270
197	254	193	192	241	420	301	308	327	258	268
303	322	299	284	291	285	285	460	257	348	308
421	266	363	309	366	426	273	308	353	315	310
308	316	277	319	348	486	285	318	333	403	295
279	313	298	176	272	254	316	320	314	335	290
329	315	300	139	303	322	318	335	302	355	375
310	235	236	236	303	302	231	364	375	378	220
313	277	307	294	252	244	340	310	347	403	276
355	314	276	335	324	253	151	203	309	235	330
354	240	350	407	391	422	382	449	449	482	375
330	254	263	315	324	349	316	263	320	384	341
351	167	204	275	329	336	360	317	83	348	358
193	142	329	305	149	180	578	387	361	133	217
253	303	381	145	191	240	251	270	127	243	174
161	174	142	127	154	209	60	259	289	237	262
139	141	228	303	213	224	248	377	191	2	279
232	319	15	125	235	163	191	234	219	161	252
223	0	292	218	273	231	263	302	186	332	32
225	175	274	116	263	284	213	277	158	207	444
308	182	242	251	258	298	294	173	200	301	142
171	405	283	218	216	213	284	257	254	183	332
292	156	344	324	233	168	258	247	183	111	332
0	255	231	244	265	323	215	153	229	270	341
168	232	321	266	265	455	186	377	351	225	209
174	12	146	363	242	296	207	258	361	466	355
283	414	294	354	158	278	266	328	219	359	195
150	265	319	398	371	384	439	289	11	177	340
207	405	140	189	317	164	136	423	298	193	248
386	216	468	428	485	521	413	685	999	303	



Table 5

ORDER	GROUP	SOURCEMS-ID	RI	EXPERIMENT	DERIVATIVE [BEST MATCH; NAME]	COMMENT	METABOLITE
1	0	SCE 189005	1888.7	1313EC36	[772; D-Glucose (5TMS)]		
2	0	SCE 272001	2723.7	1160EC23	[777; Fructose-6-phosphate methoxyamine (6TMS)]		
3	0	SCE 211003	2113.2	1313EC36	[697; Ribose-5-phosphate methoxyamine (5TMS)]		
4	0	SCE 158002	1580.7	1313EC75	[829; 1-Phenylethanol (1TMS)]		
5	0	SCE 167003	1673.2	1313EC36	[NA]		
6	0	SCE 152001	1522.3	1313EC36	Methionine (2TMS)		Methionine
7	0	SCE 151002	1509.3	1178EC16	[622; Parabanic acid (2TMS)]		
8	0	SCE 183001	1827.9	1313EC75	Arginine (5TMS)		Arginine
9	0	SCE 132003	1318.4	1313EC75	Proline (2TMS)		Proline
10	0	SCE 168004	1675.0	1274EC11	[877; Pyrophosphoric acid (4TMS)]		
11	0	SCE 277004	2770.4	1160EC15	[626; 5-Methylthioadenosine (3TMS)]		
12	0	SCE 188005	1882.4	1160EC15	Adenine (2TMS)		Adenine
13	0	SCE 283001	2826.4	1313EC75	[855; Squalene]		
14	0	SCE 189006	1892.7	1313EC36	Tyrosine (2TMS)		Tyrosine
15	0		1275.7	1135EC06	Benzoic acid (1TMS)	Contamination	Benzoic acid
16	0	SCE 148002	1481.5	1160EC15	[815; (E)-4-Methyl-5-hydroxy-3- penten-2-one (1TMS)]		
17	0		3007.7	1164EK03	5-cis-Caffeoylquinic acid (5TMS)		5-cis-Caffeoylquinic acid
18	1		3200.0	1135EC03	n-Dotriacontane		n-Dotriacontane
19	1		3600.0	1135EC04	n-Hexatriacontane		n-Hexatriacontane
20	1		2800.0	1129EC05	n-Octacosane		n-Octacosane
21	1		2200.0	1135EC03	n-Docosane		n-Docosane
22	1		1900.0	1135EC04	n-Nonadecane		n-Nonadecane
23	1		1500.0	1135EC03	n-Pentadecane		n-Pentadecane
24	1		1200.0	1135EC03	n-Dodecane		n-Dodecane

25	2	SCE	273002	2733.0	1313EC75	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	Isomaltose
26	2	SCE	291002	2906.7	1313EC75	Isomaltose methoxyamine (BP) (8TMS); alpha-D-Glc-(1,6)-D-Glc (8TMS)	
27	2	SCE	281001	2811.2	1160EC39	[895; Isomaltose methoxyamine (8TMS)]	
28	2			2836.1	1288EC38	Maltitol (9TMS); alpha-D-Glc-(1,4)-D-sorbitol (9TMS)	Maltitol
29	2	SCE	287001	2871.8	1313EC75	Isomaltose methoxyamine (8TMS); alpha-D-Glc-(1,6)-D-Glc (8TMS)	Isomaltose
30	2			2906.6	1344EC15	Isomaltose methoxyamine (BP) (8TMS); alpha-D-Glc-(1,6)-D-Glc (8TMS)	Isomaltose
31	2			2872.9	1344EC15	Isomaltose methoxyamine (8TMS); alpha-D-Glc-(1,6)-D-Glc (8TMS)	Isomaltose
32	2			2765.9	1344EC78	Maltose methoxyamine (BP) (8TMS); alpha-D-Glc-(1,4)-D-Glc	Maltose
33	2			2741.2	1344EC78	Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	Maltose
34	2			2709.9	1344EC79	Lactose methoxyamine (BP) (8TMS); beta-D-Gal-(1,4)-D-Glc	Lactose
35	2			2693.9	1344EC76	Lactose methoxyamine (8TMS); beta-D-Gal-(1,4)-D-Glc	Lactose
36	2	SCE	274002	2748.2	1274EC17	Trehalose (8TMS); alpha-D-Glc-(1,1)-alpha-D-Glc	Trehalose
37	2	SCE	262001	2619.2	1313EC75	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	
38	2	SCE	269002	2687.5	1274EC17	[964; Trehalose (8TMS); alpha-D-Glc-(1,1)-alpha-D-Glc]	

39	2	3463.2	1288EC31	Melezitose (11TMS); alpha-D-Glc-(1,3)-beta-D-Fru-(2,1)-alpha-D-Glc	Melezitose
40	2	2744.2	1288EC01	Trehalose (8TMS); alpha-D-Glc-(1,1)-alpha-D-Glc	Trehalose
41	2	2640.8	1194EK21	Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru	Sucrose
42	3	184004	1313EC36	[919; D-Xylopyranose (4TMS)]	
43	3	230001	1274EC17	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	
44	3	293001	1274EC17	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	
45	3	197002	1313EC36	[945; beta-D-Glucopyranose (5TMS)]	
46	3	181005	1274EC17	[944; D-Mannopyranose (5TMS)]	
47	3	166002	1313EC75	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	
48	3	209004	1313EC75	[756; beta-D-Methylglucopyranoside (4TMS)]	
49	3	203003	1160EC43	[766; beta-D-Methylglucopyranoside (4TMS)]	
50	3	1879.9	1344EC77	alpha-D-Methylglucopyranoside (4TMS)	alpha-D-Methylglucopyranoside
51	4	248002	1274EC17	[945; Uridine (3TMS)]	
52	4	234001	1160EC23	[882; Pseudouridine (5TMS)]	
53	4	177004	1274EC11	[812; D-Xylofuranose (4TMS)]	
54	4	209002	1313EC11	myo-Inositol (6TMS)	myo-Inositol
55	4	2091.4	1288EC40	myo-Inositol (6TMS)	myo-Inositol
56	4	179001	1313EC75	[798; Ribonic acid (5TMS)]	Gluconic acid
57	4	200001	1313EC75	Gluconic acid (6TMS)	Gluconic acid
58	4	1997.0	1288EC09	Gluconic acid (6TMS)	Galactonic acid
59	4	1991.6	2011EC38	Galactonic acid (6TMS)	Galactonic acid
60	4	1959.2	2011EC40	Gulonic acid (6TMS)	Gulonic acid



61	5	SCE	188002	1882.5	1274EC11	Mannose methoxyamine (5TMS)	Mannose
62	5	SCE	185003	1848.6	1313EC75	[708; Glucose methoxyamine (5TMS)]	
63	5	SCE	214003	2134.7	1274EC17	[904; Galactose methoxyamine (5TMS)]	
64	5	SCE	191001	1909.6	1274EC17	Glucose methoxyamine {BP} (5TMS)	Glucose
65	5	SCE	189002	1889.9	1274EC17	Glucose methoxyamine (5TMS)	Glucose
66	5	SCE	213001	2128.7	1274EC17	[857; Mannitol (6TMS)]	
67	5			1908.5	1185EK16	Glucose methoxyamine {BP} (5TMS)	Glucose
68	5			1906.6	1185EK19	Galactose methoxyamine {BP} (5TMS)	Galactose
69	5			1894.9	1185EK17	Mannose methoxyamine {BP} (5TMS)	Mannose
70	5			1889.8	1135EC00	Altrose methoxyamine (5TMS)	Altrose
71	5			1883.7	1185EK19	Galactose methoxyamine (5TMS)	Galactose
72	5			1879.8	1185EK17	Mannose methoxyamine (5TMS)	Mannose
73	6	SCE	226001	2257.2	1160EC23	[715; Erythritol (4TMS)]	
74	6	SCE	218001	2180.5	1313EC75	[733; Threitol (4TMS)]	
75	6	SCE	216003	2155.6	1313EC75	[795; Erythritol (4TMS)]	
76	6	SCE	184003	1835.3	1313EC75	[731; Erythrose (3TMS)]	
77	6	SCE	180002	1802.0	1313EC75	[706; Xylitol (5TMS)]	
78	7			1886.0	1344EC16	2-Ketogluconic acid methoxyamine {BP} (5TMS)	2-Ketogluconic acid
79	7			1869.2	1344EC16	2-Ketogluconic acid methoxyamine (5TMS)	2-Ketogluconic acid
80	7			1862.2	2011EC39	2-Keto-L-gulonic acid methoxyamine (5TMS)	2-Keto-L-gulonic acid
81	7	SCE	188004	1879.6	1313EC75	Fructose methoxyamine {BP} (5TMS)	Fructose
82	7	SCE	187002	1869.1	1313EC75	Fructose methoxyamine (5TMS)	Fructose

83	7	1875.4	1185EK18	Fructose methoxyamine {BP} (5TMS)	Fructose
84	7	1870.1	1135EC00	Sorbose methoxyamine {BP} (5TMS)	Sorbose
85	7	1866.7	1185EK18	Fructose methoxyamine (5TMS)	Fructose
86	7	1865.3	1135EC00	Sorbose methoxyamine (5TMS)	Sorbose
87	7	1670.8	1313EC75	Arabinose methoxyamine (4TMS)	Arabinose
88	7	1681.9	1288EC26	Ribose methoxyamine (4TMS)	Ribose
89	7	1666.9	1288EC25	Arabinose methoxyamine (4TMS)	Arabinose
90	7	1660.4	1288EC27	Xylose methoxyamine (4TMS)	Xylose
91	7	1652.8	1288EC27	Xylose methoxyamine {BP} (4TMS)	Xylose
92	8	1956.6	1313EC75	[793; D-Galactono-1,4-lactone (4TMS)]	
93	8	2766.5	1135EC00	Turanose methoxyamine {BP} (8TMS); alpha-D-Glc-(1,3)-D-Fru	Turanose
94	8	2744.4	1135EC00	Turanose methoxyamine (8TMS); alpha-D-Glc-(1,3)-D-Fru	Turanose
95	8	1921.2	2011EC40	D(-)-Gulono-1,4-lactone (4TMS)	D(-)-Gulono-1,4-lactone
96	8	1920.6	2011EC41	L(+)-Gulono-1,4-lactone (4TMS)	L(+)-Gulono-1,4-lactone
97	8	1886.5	2011EC38	L(+)-Galactono-1,4-lactone (4TMS)	L(+)-Galactono-1,4-lactone
98	8	1884.8	2011EC37	D(-)-Galactono-1,4-lactone (4TMS)	D(-)-Galactono-1,4-lactone
99	8	1710.6	1274EC17	[817; Ribitol (5TMS)]	Erythritol
100	8	1502.4	1288EC34	Erythritol (4TMS)	Sorbitol
101	8	1931.9	1313EC75	Sorbitol (6TMS); Glucitol (6TMS)	
102	8	1924.2	1313EC57	Mannitol (6TMS)	Mannitol

103	8	1931.1	1288EC35	Sorbitol (6TMS); Glucitol (6TMS)	Sorbitol
104	8	1927.7	1288EC32	Mannitol (6TMS)	Mannitol
105	8	1731.5	1313EC36	Ribitol (5TMS)	Ribitol
106	8	1726.6	1135EC25	Ribitol (5TMS)	Ribitol
107	8	1935.5	1288EC36	Galactitol (6TMS)	Galactitol
108	8	1710.0	1288EC37	Xylitol (5TMS)	Xylitol
109	8	1503.9	1313EC75	Erythritol (4TMS)	Erythritol
110	8	1494.1	1135EC00	Threitol (4TMS)	Threitol
111	9	3152.5	1164EK03	1-Caffeoylquinic acid (BP)	1-trans-Caffeoylquinic acid
112	9	3138.7	1164EK03	4-Caffeoylquinic acid (BP)	
113	9	3397.0	1164EK03	1-trans-Caffeoylquinic acid (6TMS)	
114	9	3168.3	1164EK03	4-trans-Caffeoylquinic acid (6TMS)	
115	9	3009.1	1164EK03	4-cis-Caffeoylquinic acid (6TMS)	4-cis-Caffeoylquinic acid
116	9	3190.0	1164EK03	5-trans-Caffeoylquinic acid (6TMS)	5-trans-Caffeoylquinic acid
117	9	3113.7	1164EK03	3-trans-Caffeoylquinic acid (6TMS)	3-trans-Caffeoylquinic acid
118	9	2990.3	1164EK03	3-cis-Caffeoylquinic acid (6TMS)	3-cis-Caffeoylquinic acid
119	10	2014.0	1288EC06	Glucaric acid (6TMS)	Glucaric acid
120	10	1961.3	1288EC07	Galacturonic acid methoxyamine (BP) (5TMS)	Galacturonic acid
121	10	1940.3	1288EC07	Galacturonic acid methoxyamine (5TMS)	Galacturonic acid
122	10	1723.7	1160EC15	2-Aminoadipic acid (3TMS)	2-Aminoadipic acid
123	10	2089.0	1288EC05	Allantoin (3TMS)	Allantoin
124	10	2775.3	1344EC07	Guanosine (5TMS)	Guanosine
125	10	2727.0	1344EC26	Adenosine (4TMS)	Adenosine
126	10	2660.0	1135EC00	Xanthosine (5TMS)	Xanthosine
127	10	1853.9	1164EK02	Dehydroascorbic acid dimer; L(+)-Ascorbic acid (BP)	Dehydroascorbic acid dimer; L(+)-Ascorbic acid
128	10	1826.9	1313EC200	Citric acid (4TMS)	Citric acid

129	10	1821.6	1288EC03	Isocitric acid (4TMS)	Isocitric acid
130	10	1854.9	1164EK03	D(-)-Quinic acid (5TMS)	D(-)-Quinic acid
131	10	1813.5	1313EC199	Shikimic acid (4TMS)	Shikimic acid
132	10	SCE 175003	1313EC36	[612; 4-Aminobutyric acid (2TBS)]	
133	10	SCE 176004	1313EC75	[757; 2-Desoxy-pentos-3-ylose dimethoxyamine (2TMS)]	
134	10	SCE 169001	1313EC75	[746; Ribonic acid-1,4-lactone (3TMS)]	
135	10	SCE 137001	1313EC75	Fumaric acid (2TMS)	Fumaric acid
136	10	1372.0	1288EC46	Fumaric acid (2TMS)	Fumaric acid
137	10	1759.0	1344EC20	cis-Aconitic acid (3TMS)	cis-Aconitic acid
138	10	1608.3	2011EC27	2-Ketoglutaric acid methoxyamine (2TMS)	2-Ketoglutaric acid
139	10	SCE 192007	1313EC57	[761; 2-Hydroxy-3-methyl-2-butenic acid (2TBS)]	
140	10	SCE 182004	1313EC75	Citric acid (4TMS)	Citric acid
141	10	SCE 158003	1274EC17	[680; 2,3-Dimethylsuccinic acid (2TMS)]	
142	10	SCE 157002	1274EC17	[708; 2,3-Dimethylsuccinic acid (2TMS)]	
143	10	SCE 127002	1135EC44	Urea (2TMS)	Urea
144	10	1428.7	1344EC11	Glutaric acid (2TMS)	Glutaric acid
145	10	SCE 148001	1313EC75	Citramalic acid (3TMS)	Citramalic acid
146	10	1475.1	1288EC45	Citramalic acid (3TMS)	Citramalic acid
147	10	SCE 134001	1313EC75	Succinic acid (2TMS)	Succinic acid
148	10	1346.0	2011EC29	Succinic acid (2TMS)	Succinic acid
149	10	SCE 127005	1313EC43	[938; Sulfuric acid (2TMS)]	
150	10	SCE 146003	1313EC75	[725; 2-Ketooctanoic acid (2TMS)]	
151	10	1373.5	1164CC54	2-Methyl-2-butenedioic acid (2TMS)	2-Methyl-2-butenedioic acid
152	10	1336.4	2011EC31	Maleic acid (2TMS)	Maleic acid
153	11	SCE 258001	1274EC11	[734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]	

154	11	SCE	174002	1735.8	1313EC75	Glycerol-2-phosphate (4TMS)	Glycerol-2-phosphate
155	11	SCE	217002	2168.9	1313EC75	[705; 2-Ketogluconic acid (5TMS)]	
156	11			1730.5	1288EC39	Rhamnose methoxyamine {BP} (4TMS)	Rhamnose
157	11			1745.0	1288EC30	Fucose methoxyamine {BP} (4TMS)	Fucose
158	11			1731.6	1288EC30	Fucose methoxyamine (4TMS)	Fucose
159	11			1722.2	1288EC39	Rhamnose methoxyamine (4TMS)	Rhamnose
160	11	SCE	140003	1394.9	1274EC17	[644; 2-Methyl-1,3-butanediol (2TMS)]	
161	11			1412.3	1344EC09	Lactic acid dimer (2TMS)	Lactic acid forms lactic acid dimer
162	11	SCE	266001	2656.9	1313EC75	[559; Erythritol (4TMS)]	
163	11	SCE	228001	2278.6	1274EC17	[583; Erythritol (4TMS)]	
164	11	SCE	252002	2518.0	1313EC75	[644; Erythritol (4TMS)]	
165	11	SCE	249001	2493.1	1313EC75	[657; Erythritol (4TMS)]	
166	11	SCE	180001	1796.4	1313EC75	[646; 3-Deoxyglucitol (5TMS)]	
167	11			1957.4	1164EK02	D(-)-Isoascorbic acid (4TMS)	D(-)-Isoascorbic acid
168	11			1946.4	1164EK02	L(+)-Ascorbic acid (4TMS)	L(+)-Ascorbic acid
169	11	SCE	135003	1352.5	1274EC17	Glyceric acid (3TMS)	Glyceric acid
170	11			1639.3	1135EC00	Tartaric acid (4TMS); 2,3-Dihydroxybutanedioic acid (4TMS)	Tartaric acid
171	11	SCE	154001	1544.5	1313EC75	Erythronic acid (4TMS)	Erythronic acid
172	11			1559.6	2011EC33	Threonic acid (4TMS)	Threonic acid
173	11	SCE	149001	1488.2	1274EC17	Malic acid (3TMS)	Malic acid
174	11			1488.5	1288EC44	Malic acid (3TMS)	Malic acid
175	11	SCE	238002	2383.7	1313EC75	[724; Glycerol (3TMS)]	
176	11	SCE	173002	1726.7	1313EC36	Fucose methoxyamine (4TMS)	Fucose
177	11			1461.7	1135EC00	Threose methoxyamine {BP} (3TMS)	Threose
178	11			1467.9	1135EC00	Threose methoxyamine (3TMS)	Threose
179	11			1464.3	1344EC12	Erythrose methoxyamine (3TMS)	Erythrose

180	11	1453.0	1344EC12	Erythrose methoxyamine {BP} (3TMS)	Erythrose
181	11	1293.1	1313EC75	Glycerol (3TMS)	Glycerol
182	11	1302.8	2011EC21	Glycerol (3TMS)	Glycerol
183	12	2109.7	1313EC75	[662; Ribose-5-phosphate methoxyamine {BP} (5TMS)]	
184	12	2427.1	1274EC17	[931; myo-Inositol-2-phosphate (7TMS)]	
185	12	3183.2	1160EC23	[748; D-Sedoheptulose-7- phosphate (7TMS)]	
186	12	2386.9	1160EC23	[928; Glucopyranose-6-phosphate (6TMS)]	
187	12	2383.0	2011EC24	Sorbitol-6-phosphate (7TMS)	Sorbitol-6-phosphate
188	12	2320.2	1191EC10	Fructose-6-phosphate methoxyamine (6TMS)	Fructose-6-phosphate
189	12	2679.2	1160EC23	[837; alpha-D-Fructofuranose-1,6- bisphosphate (7TMS)]	
190	12	2474.0	1344EC24	myo-Inositol-2-phosphate (7TMS)	myo-Inositol-2-phosphate
191	12	2718.4	1313EC43	[824; D-Sedoheptulose-7- phosphate (7TMS)]	
192	12	2318.9	2011EC23	Fructose-6-phosphate methoxyamine (6TMS)	Fructose-6-phosphate
193	12	2564.4	1313EC75	[945; Galactofuranose-6-phosphate (7TMS)]	
194	12	2347.2	1313EC43	Glucose-6-phosphate methoxyamine {BP} (6TMS)	Glucose-6-phosphate
195	12	2328.1	1313EC75	Glucose-6-phosphate methoxyamine (6TMS)	Glucose-6-phosphate
196	12	2440.4	2011EC32	Gluconic acid-6-phosphate (7TMS)	Gluconic acid-6-phosphate
197	12	2350.9	2011EC22	Glucose-6-phosphate methoxyamine {BP} (6TMS)	Glucose-6-phosphate
198	12	2348.0	1344EC17	Galactose-6-phosphate methoxyamine {BP} (6TMS)	Galactose-6-phosphate
199	12	2330.5	2011EC22	Glucose-6-phosphate methoxyamine (6TMS)	Glucose-6-phosphate

200	12	2311.4	1344EC17	Galactose-6-phosphate methoxyamine (6TMS)	Galactose-6-phosphate
201	12	2331.8	1344EC18	Mannose-6-phosphate methoxyamine (BP) (6TMS)	Mannose-6-phosphate
202	12	2313.9	1344EC18	Mannose-6-phosphate methoxyamine (6TMS)	Mannose-6-phosphate
203	12	3080.1	1160EC23	[808; Adenosine-5-monophosphate (5TMS)]	
204	12	2023.7	1274EC17	[680; Glycerol-2-phosphate (4TMS)]	
205	12	1813.0	1313EC75	Glyceric acid-3-phosphate (4TMS)	Glyceric acid-3-phosphate
206	12	1813.4	1344EC13	Glyceric acid-3-phosphate (4TMS)	Glyceric acid-3-phosphate
207	12	1769.9	1313EC75	Glycerol-3-phosphate (4TMS)	Glycerol-3-phosphate
208	12	1770.0	1344EC63	L-Glycerol-3-phosphate (4TMS)	L-Glycerol-3-phosphate
209	12	1735.8	1344EC63	L-Glycerol-2-phosphate (4TMS)	L-Glycerol-2-phosphate
210	12	1731.7	1344EC71	DL-Glyceraldehyde-3-phosphate methoxyamine (BP) (3TMS)	DL-Glyceraldehyde-3- phosphate
211	12	1719.5	1344EC71	DL-Glyceraldehyde-3-phosphate methoxyamine (3TMS)	DL-Glyceraldehyde-3- phosphate
212	12	1723.3	1344EC71	DL-Glyceraldehyde-3-phosphate methoxyamine (BP) (3TMS)	DL-Glyceraldehyde-3- phosphate
213	12	1708.9	1344EC71	DL-Glyceraldehyde-3-phosphate methoxyamine (BP) (3TMS)	DL-Glyceraldehyde-3- phosphate
214	12	2311.4	1274EC17	Galactose-6-phosphate methoxyamine (6TMS)	Galactose-6-phosphate
215	12	1296.5	1191EC10	Phosphoric acid (3TMS)	Phosphoric acid
216	12	1293.1	1164EK02	Phosphoric acid (3TMS)	Phosphoric acid
217	13	2651.1	1160EC15	[721; Adenosine (4TMS)]	

218	13	SCE	181004	1806.2	1313EC75	[549; 2-Keto-D-gluconic acid (5TMS)]	alpha-D-Methylglucopyranoside (4TMS)
219	13	SCE	188006	1877.4	1274EC17		
220	13	SCE	138001	1381.0	1313EC75	Serine (3TMS)	Serine
221	14	SCE	177003	1770.3	1274EC17	[NA]	
222	14	SCE	179002	1794.4	1274EC17	[789; Tyramine (3TMS)]	
223	14	SCE	143003	1436.0	1313EC36	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	
224	14	SCE	128002	1281.5	1313EC36	Ethanolamine (3TMS)	Ethanolamine
225	14	SCE	216002	2162.3	1313EC75	[648; Ethylamine (2TMS)]	
226	14	SCE	154002	1538.2	1313EC36	[596; N-Acetylglutamic acid (2TMS)]	
227	14	SCE	192003	1915.4	1274EC17	Lysine (4TMS)	Lysine
228	14			1916.6	1164EK04	L-Lysine (4TMS)	L-Lysine
229	14	SCE	186002	1858.1	1313EC36	Lysine (3TMS)	Lysine
230	14	SCE	200002	2002.2	1178EC16	[775; Dopamine (4TMS)]	
231	14	SCE	176006	1763.9	1313EC75	Ornithine (3TMS); Arginine {BP} (3TMS)	Ornithine; Arginine
232	14			2255.2	1344EC14	Spermidine (5TMS)	Spermidine
233	14			2197.4	1344EC14	Spermidine (4TMS) {BP}	Spermidine
234	14	SCE	182002	1819.8	1313EC75	Ornithine (4TMS); Arginine {BP} (4TMS)	Ornithine; Arginine
235	14			1820.5	1185EK04	Ornithine (4TMS)	Ornithine; Arginine
236	14			1412.9	1164EK04	O-Acetyl-L-serine (2TMS)	O-Acetyl-L-serine
237	14			2075.8	2011EC34	Dopamine (4TMS)	Dopamine
238	14			1914.2	2011EC35	Tyramine (3TMS)	Tyramine
239	14	SCE	206001	2064.0	1191EC10	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	
240	14			1737.0	1135EC00	6-Aminocaproic acid (3TMS)	6-Aminocaproic acid
241	14			1636.7	1135EC00	5-Aminovaleric acid (3TMS)	5-Aminovaleric acid
242	14	SCE	213003	2125.3	1313EC75	[832; Dopamine (4TMS)]	
243	14	SCE	133001	1326.5	1274EC17	Glycine (3TMS)	Glycine
244	14			1533.6	1344EC21	4-Aminobutyric acid (3TMS)	4-Aminobutyric acid
245	14			1440.4	1185EK03	beta-Alanine (3TMS)	beta-Alanine



246	14				1326.9	1185EK07	Glycine (3TMS)	Glycine
247	15	SCE	340002		3401.9	1274EC11	[805; 4,4-Dimethylcholesta-8,24-dien-3-ol (1TMS)]	
248	15	SCE	334001		3337.9	1191EC10	[700; Ergosta-5,7-dien-3-ol]	
249	15	SCE	331001		3301.9	1274EC11	[674; Ergosterol (1TMS)]	
250	15	SCE	327001		3270.3	1313EC36	Ergosterol (1TMS)	Ergosterol
251	15	SCE	338001		3380.0	1274EC11	Lanosta-8,24-dien-3-beta-ol (1TMS)	Lanosta-8,24-dien-3-beta-ol
252	15	SCE	335001		3350.3	1274EC11	[692; Ergosta-7,22-dien-3-ol (1TMS)]	
253	15				3374.5	2014EC05	Stigmastan-3-ol (1TMS)	
254	15	SCE	349001		3487.5	1191EC08	[568; 2,3-Dihexadecanoylglycerol (1TMS)]	Stigmastan-3-ol
255	15	SCE	223003		2225.2	1313EC36	Octadecenoic acid (1TMS)	Octadecenoic acid
256	15	SCE	222001		2217.8	1274EC17	9-(Z)-Octadecenoic acid (1TMS)	9-(Z)-Octadecenoic acid
257	15	SCE	203002		2029.2	1274EC17	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	
258	15	SCE	225002		2245.5	1313EC75	Octadecanoic acid (1TMS)	Octadecanoic acid
259	15	SCE	205001		2048.2	1313EC75	Hexadecanoic acid (1TMS)	Hexadecanoic acid
260	15	SCE	185004		1850.9	1274EC11	[912; Tetradecanoic acid (1TMS)]	
261	15				2834.5	1180EC112	Tetracosanoic acid (1TMS)	Tetracosanoic acid
262	16				3296.6	1164EK03	1-Caffeoylquinic acid (BP)	
263	16				2139.0	1164EK03	trans-Caffeic acid (3TMS)	trans-Caffeic acid
264	16				1985.5	1164EK03	cis-Caffeic acid (3TMS)	cis-Caffeic acid
265	16				2253.1	1164EK03	trans-Sinapinic acid (2TMS)	trans-Sinapinic acid
266	16				2066.6	1164EK03	cis-Sinapinic acid (2TMS)	cis-Sinapinic acid
267	16				2101.9	1164EK03	trans-Ferulic acid (2TMS)	trans-Ferulic acid
268	16				1947.0	2011EC48	trans-p-Coumaric acid (2TMS)	trans-p-Coumaric acid
269	16				1924.7	1164EK03	cis-Ferulic acid (2TMS)	cis-Ferulic acid
270	16				1821.6	2011EC49	trans-o-Coumaric acid (2TMS)	trans-o-Coumaric acid
271	17	SCE	223001		2225.6	1178EC20	Tryptophan (2TMS)	Tryptophan
272	17				2225.2	1179EK02	L-Tryptophan (2TMS)	L-Tryptophan
273	17				2226.4	1164EK04	L-Tryptophan (3TMS)	L-Tryptophan
274	17				1975.9	1344EC27	Indole3-acetic acid (2TMS)	Indole3-acetic acid

275	17	SCE	151003	1514.1	1313EC36	[729; N,N-Dimethyllysine methyl ester]	L-Asparagine
276	17			1871.6	1164EK04	L-Asparagine (4TMS)	
277	17	SCE	174003	1739.1	1274EC11	[NA]	
278	17	SCE	141003	1410.5	1313EC75	[700; 2-methyl-1,2-propanediol (2TMS)]	
279	17	SCE	192006	1924.5	1313EC16	Histidine (3TMS)	Histidine
280	17	SCE	187004	1868.5	1274EC17	[826; beta-[[[5-methyl-2-thienyl)methyleneamino-benzeneacetic acid methyl ester]	
281	17	SCE	184002	1842.1	1313EC75	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	
282	17	SCE	176003	1755.7	1313EC75	[829; Orotic acid (3TMS)]	
283	17	SCE	136001	1364.2	1313EC11	Uracil (2TMS)	Uracil
284	17			1419.2	1135EC00	Thymine (2TMS)	Thymine
285	17	SCE	204003	2039.0	1313EC43	[607; Putrescine (4TMS)]	
286	17	SCE	172005	1720.9	1313EC36	[NA]	
287	17	SCE	150003	1495.6	1313EC36	[815; Ethyl-3(2H)-thiophenone]	
288	17	SCE	167001	1673.8	1191EC10	Homocysteine (3TMS)	Homocysteine
289	17	SCE	141004	1414.0	1274EC17	[590; 1-Acetyl-2-thiohydantoin]	
290	17			1940.4	1344EC27	Indole-3-acetic acid (1TMS)	Indole-3-acetic acid
291	17	SCE	157001	1565.1	1274EC17	Phenylalanine (1TMS)	Phenylalanine
292	17			1565.2	1164EK04	L-Phenylalanine (1TMS)	L-Phenylalanine
293	17	SCE	335002	3358.2	1191EC08	[693; Ergost-7-en-3-ol (1TMS)]	
294	17	SCE	182006	1824.3	1191EC08	[570; Hypoxanthine (2TMS)]	
295	17			1908.3	1344EC04	Adenine (1TMS)	Adenine
296	17			1879.6	1344EC04	Adenine (2TMS)	Adenine
297	17			2911.5	1344EC10	delta-Tocopherol (1TMS)	delta-Tocopherol
298	17			1843.5	2011EC47	p-Aminobenzoic acid (2TMS)	p-Aminobenzoic acid
299	17			1628.2	1344EC22	Anthranilic acid (2TMS)	Anthranilic acid
300	17			2233.1	1313EC75	n-Nonadecanoic acid methyl ester	n-Nonadecanoic acid methyl ester
301	17			1402.9	1344EC19	Mevalonic acid-1,5-lactone (1TMS)	Mevalonic acid-1,5-lactone
302	18	SCE	132002	1316.0	1313EC36	Isoleucine (2TMS)	Isoleucine
303	18			1315.1	1164EK04	L-Isoleucine (2TMS)	L-Isoleucine

304	18			1351.6	1344EC23	Norleucine (2TMS)	Norleucine
305	18	SCE	129002	1291.0	1185EK01	Leucine (2TMS)	Leucine
306	18	SCE	129002	1291.0	1185EK01	Leucine (2TMS)	Leucine
307	18	SCE	159001	1595.8	1274EC17	[639; Proline (2TMS)]	
308	18			1318.8	1185EK05	L-Proline (2TMS)	L-Proline
309	18	SCE	163001	1625.9	1274EC17	Glutamic acid (3TMS)	Glutamic acid
310	18			1627.1	1185EK12	L-Glutamic acid (3TMS)	L-Glutamic acid
311	18	SCE	178001	1784.4	1313EC36	Glutamine (3TMS)	Glutamine
312	18			1782.6	1185EK08	L-Glutamine (3TMS)	L-Glutamine
313	18	SCE	153002	1529.0	1313EC75	Pyroglutamic acid (2TMS)	Pyroglutamic acid
314	18			1530.9	1185EK13	Pyroglutamic acid (2TMS)	Pyroglutamic acid
315	18			1526.0	1185EK10	4-Hydroxyproline (3TMS)	4-Hydroxyproline
316	18	SCE	165002	1653.8	1191EC10	[548; Leucine (2TBS)]	
317	18	SCE	171003	1708.2	1313EC36	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	
318	18	SCE	176005	1758.1	1313EC75	[636; 4R-Acetalamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	
319	18			2135.1	1344EC07	Guanine (4TMS)	Guanine
320	18			2086.8	1344EC29	Prephenic acid methoxyamine (3TMS)	Prephenic acid
321	18			1630.2	1135EC00	Triethanolamine (3TMS)	Triethanolamine
322	18			2127.8	2011EC19	L(+)-Cystathionine (2TMS)	L(+)-Cystathionine
323	18			1140.2	1185EK07	Glycine (2TMS)	Glycine
324	18			1456.9	1164EK04	L-Homoserine (3TMS)	L-Homoserine
325	18	SCE	140001	1403.1	1274EC17	Threonine (3TMS)	Threonine
326	18			1402.5	1164EK04	L-Threonine (3TMS)	L-Threonine
327	18	SCE	146001	1459.3	1313EC36	Homoserine (3TMS)	Homoserine
328	18			2206.1	1164EK04	L(+)-Cystathionine (4TMS)	L(+)-Cystathionine
329	18			1674.4	1164EK04	DL-Homocysteine (3TMS)	DL-Homocysteine
330	18			2174.2	2011EC19	L(+)-Cystathionine (BP) (3TMS)	L(+)-Cystathionine
331	18			1523.1	1164EK04	L-Methionine (2TMS)	L-Methionine
332	18	SCE	156002	1560.7	1191EC08	Cysteine (3TMS)	Cysteine
333	18			1560.6	1164EK04	L-Cysteine (3TMS)	L-Cysteine
334	18	SCE	194002	1938.9	1274EC17	Tyrosine (3TMS)	Tyrosine
335	18			1939.9	1185EK11	L-Tyrosine (3TMS)	L-Tyrosine

336	18	SCE	164001	1640.8	1313EC36	Phenylalanine (2TMS)	Phenylalanine
337	18			1641.7	1164EK04	L-Phenylalanine (2TMS)	L-Phenylalanine
338	18			1441.4	1344EC30	S-Methylcysteine (2TMS)	S-Methylcysteine
339	18			1380.3	1164EK04	L-Serine (3TMS)	L-Serine
340	18	SCE	138002	1378.1	1313EC75	Alanine (3TMS)	Alanine
341	18			1379.5	1185EK02	L-Alanine (3TMS)	L-Alanine
342	18	SCE	168001	1682.1	1160EC15	Asparagine (3TMS)	Asparagine
343	18			1681.2	1164EK04	L-Asparagine (3TMS)	L-Asparagine
344	18			1510.5	1164EK04	N-Acetyl-L-serine (2TMS)	N-Acetyl-L-serine
345	18	SCE	152002	1520.6	1313EC75	Aspartic acid (3TMS)	Aspartic acid
346	18			1519.2	1185EK09	L-Aspartic acid (3TMS)	L-Aspartic acid
347	18			1334.7	1344EC21	4-Aminobutyric acid (2TMS)	4-Aminobutyric acid
348	18	SCE	162001	1623.5	1313EC36	[882; Ornithine (3TMS)]	
349	18	SCE	147002	1474.4	1191EC10	[NA]	
350	18	SCE	147003	1467.9	1178EC16	[709; 2,5-Diaminovalerolactam (2TMS)]	
351	18			1260.4	2011EC44	Norvaline (2TMS)	Norvaline
352	18	SCE	122001	1220.2	1274EC17	Valine (2TMS)	Valine
353	18			1221.9	1185EK06	L-Valine (2TMS)	L-Valine
354	18	SCE	144007	1450.0	1313EC75	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	
355	18	SCE	132001	1317.6	1313EC75	Threonine (2TMS)	Threonine
356	18			1318.9	1164EK04	L-Threonine (2TMS)	L-Threonine
357	18	SCE	144003	1440.3	1274EC17	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	
358	18	SCE	142001	1419.8	1313EC75	Alanine {BP} (3TMS)	
359	18	SCE	128001	1282.1	1274EC17	Serine (2TMS)	Serine
360	18			1280.9	1164EK04	L-Serine (2TMS)	L-Serine
361	18			1102.5	1185EK02	L-Alanine (2TMS)	L-Alanine





ID	METABOLITE	MS/MS (MS-ID)	FRAGMENTS [M/Z, RI]	MEOH.S74	MEOH.S75	MEOH.S76	MEOH.S77	MEOH.S78	MEOH.S79	MEOH.S80	MEOH.S81	MEOH.S82	MEOH.S83	MEOH.S84	MEOH.S85	MEOH.S86	MEOH.S87	MEOH.S88	MEOH.S89
125	[82; Sucrose (RTMS); alpha-D-Glc-(1-2)-beta-D-Fru]	262001	(361 + 73)_2620	4.1434	6.1097	11.2150	11.0168	8.8608	12.4702	11.8464	6.1149	6.7381	8.9506	9.3997	8.1072	6.6999	13.4941	16.3584	8.6946
126	[58; Erythritol (RTMS)]	260001	(73 + 127)_2657	0.2308	0.2770	0.1629	0.1650	0.3838	0.1917	0.2903	0.4494	0.2839	0.2651	0.1931	0.8981	0.3016	0.2375	0.1399	0.2412
127	[77; Fructose-6-phosphate methylxanthine (RTMS)]	270001	(387 + 315)_2726	0.1257	0.1681	0.1138	0.1341	0.0823	0.0836	0.0940	0.1933	0.1547	0.1705	0.2083	0.2338	0.2028	0.1741	0.1078	0.1282
128	[82; D-Sedoheptulose-7-phosphate (RTMS)]	270002	(73 + 315)_2721	0.3181	0.3416	0.3163	0.3769	0.0899	0.1054	0.1360	0.3843	0.1971	0.3588	0.4403	0.4805	0.4374	0.3454	0.0934	0.2740
129	[84; Mannose methylxanthine (RTMS); alpha-D-Glc-(1,4)-D-Glc]	270003	(204 + 180)_2734	0.2454	0.3988	0.2702	0.4078	0.2810	0.1993	0.3186	0.3265	0.4024	0.2388	0.2324	0.4193	0.2707	0.1952	0.0934	0.2740
130	Trehalose	270004	(183 + 189)_2747	2.1363	4.8237	4.5907	5.2090	5.1317	2.4086	2.7579	3.3884	3.6987	4.2238	3.3937	2.8213	3.4943	3.5909	2.7889	3.3937
131	[82; 5-Hydroxythiadenosine (RTMS)]	277004	(194)_2770	0.0053	0.0076	0.0159	0.0142	0.0057	0.0053	0.0053	0.0053	0.0053	0.0051	0.0047	0.0038	0.0028	0.0028	0.0028	0.0052
132	[85; Mannose methylxanthine (RTMS)]	281001	(204)_2817	0.0802	0.0290	0.0812	0.0837	0.0393	0.1125	0.1038	0.1334	0.0963	0.1161	0.1126	0.0903	0.1209	0.1320	0.1487	0.1007
133	[85; Squaraine]	283001	(84 + 81)_2830	0.2487	0.2084	0.1708	0.2076	0.1916	0.2602	0.2834	0.1334	0.1883	0.2999	0.4318	0.2914	0.3434	0.2581	0.2835	0.3703
134	Isomaltose	287001 and 281002	(381 + 73)_2872 and (73 + 381)_2908	2.1824	0.0221	5.3599	6.1864	4.3059	3.2447	4.3948	6.2330	6.6992	4.4867	4.3154	6.8497	3.9709	4.1978	3.9162	4.3987
135	[82; Mannose (RTMS); alpha-D-Glc-(1,6)-D-Glc (RTMS)]	293001	(204)_2932	0.0724	0.3237	0.3132	0.3417	0.2618	0.3878	0.4594	0.3481	0.3754	0.5017	0.527	0.2345	0.2709	0.1930	0.0538	0.4879
136	[74; D-Galactose-7-phosphate (RTMS)]	318001	(315 + 73)_3188	0.3516	0.0530	0.0530	0.0530	0.0530	0.0530	0.0530	0.0530	0.0530	0.0530	0.0530	0.0530	0.0530	0.0530	0.0530	0.0530
137	Ergosterol	327001	(317 + 61)_3270	0.5898	0.5383	0.5704	0.4928	0.4609	0.4351	0.8025	0.4825	0.5002	0.9507	0.8881	0.7418	0.9468	1.0137	0.9870	0.8885
138	[874; Ergosterol (RTMS)]	331001	(145 + 120)_3311	0.0323	0.0187	0.0196	0.0140	0.0105	0.0311	0.0307	0.0141	0.0154	0.0402	0.0537	0.0377	0.0408	0.0475	0.0475	0.0539
139	[700; Ergosterol-7,22-dim-3-ol]	334001	(79)_3349	0.0090	0.0049	0.0040	0.0074	0.0074	0.0074	0.0074	0.0074	0.0074	0.0074	0.0074	0.0074	0.0074	0.0074	0.0074	0.0074
140	[892; Ergosterol-7,22-dim-3-ol (RTMS)]	335001	(79)_3349	0.0220	0.0119	0.0188	0.0169	0.0149	0.0231	0.0231	0.0231	0.0231	0.0231	0.0231	0.0231	0.0231	0.0231	0.0231	0.0231
141	Lanosterol-4,24-dim-3-bis-ol	338001	(65 + 120)_3382	0.0460	0.0372	0.0450	0.0365	0.0344	0.0580	0.0577	0.0347	0.0414	0.0716	0.0738	0.0591	0.0685	0.0291	0.0260	0.0262







[illegible]











ID	METABOLITE	MSTs [MS-ID]	FRAGMENTS (M/Z), R1	FILTER.S56	FILTER.S57	FILTER.S58	FILTER.S59	FILTER.S60	FILTER.S61	FILTER.S62	FILTER.S63	FILTER.S64	FILTER.S66	FILTER.S67	FILTER.S68	FILTER.S69	FILTER.S70	FILTER.S71	FILTER.S72	
123	[82] Sucrose (RTMS); alpha-D-Glc-(1,2)-beta-D-Fru	262001	(81 + 73), 2820	124528	10.2181	0.0238	0.0289	0.0238	5.3888	4.3023	5.1885	5.7561	7.4709	8.8304	8.8958	5.732	5.9918	5.7752	5.2823	4.8478
126	[55] Erythritol (RTMS)	265001	(73 + 127), 2557	0.0238	0.0289	0.0238	0.0289	0.0238	5.3888	4.3023	5.1885	5.7561	7.4709	8.8304	8.8958	5.732	5.9918	5.7752	5.2823	4.8478
127	[77] Fructose-6-phosphate methylcarbamate (RTMS)	272001	(57 + 315), 2726	0.0238	0.0289	0.0238	0.0289	0.0238	5.3888	4.3023	5.1885	5.7561	7.4709	8.8304	8.8958	5.732	5.9918	5.7752	5.2823	4.8478
128	[82] D-Sedoheptulose-7-phosphate (RTMS)	273002	(73 + 315), 2721	0.0238	0.0289	0.0238	0.0289	0.0238	5.3888	4.3023	5.1885	5.7561	7.4709	8.8304	8.8958	5.732	5.9918	5.7752	5.2823	4.8478
129	[82] Malbise methylcarbamate (RTMS); alpha-D-Glc-(1,4)-D-Glc	273002	(204 + 169), 2734	0.0238	0.0289	0.0238	0.0289	0.0238	5.3888	4.3023	5.1885	5.7561	7.4709	8.8304	8.8958	5.732	5.9918	5.7752	5.2823	4.8478
130	Trehalose	274002	(163 + 169), 2747	0.0238	0.0289	0.0238	0.0289	0.0238	5.3888	4.3023	5.1885	5.7561	7.4709	8.8304	8.8958	5.732	5.9918	5.7752	5.2823	4.8478
131	[82] 5-Methylglucosamine (RTMS)	277004	(164), 2770	0.0238	0.0289	0.0238	0.0289	0.0238	5.3888	4.3023	5.1885	5.7561	7.4709	8.8304	8.8958	5.732	5.9918	5.7752	5.2823	4.8478
132	[82] Isomaltose methylcarbamate (RTMS)	281001	(204), 2817	0.0238	0.0289	0.0238	0.0289	0.0238	5.3888	4.3023	5.1885	5.7561	7.4709	8.8304	8.8958	5.732	5.9918	5.7752	5.2823	4.8478
133	[85] Squalene	283001	(84 + 81), 2830	0.0238	0.0289	0.0238	0.0289	0.0238	5.3888	4.3023	5.1885	5.7561	7.4709	8.8304	8.8958	5.732	5.9918	5.7752	5.2823	4.8478
134	Isomaltose	287001 and 281002	(361 + 73), 2872 and (73 + 361), 2808	0.0238	0.0289	0.0238	0.0289	0.0238	5.3888	4.3023	5.1885	5.7561	7.4709	8.8304	8.8958	5.732	5.9918	5.7752	5.2823	4.8478
135	[82] Melibiose (RTMS); alpha-D-Glc-(1,6)-D-Glc (RTMS)	293001	(204), 2932	0.0238	0.0289	0.0238	0.0289	0.0238	5.3888	4.3023	5.1885	5.7561	7.4709	8.8304	8.8958	5.732	5.9918	5.7752	5.2823	4.8478
136	[74] D-Sedoheptulose-7-phosphate (RTMS)	318001	(315 + 73), 3188	0.0238	0.0289	0.0238	0.0289	0.0238	5.3888	4.3023	5.1885	5.7561	7.4709	8.8304	8.8958	5.732	5.9918	5.7752	5.2823	4.8478
137	Ergosterol	327001	(337 + 81), 3270	0.0238	0.0289	0.0238	0.0289	0.0238	5.3888	4.3023	5.1885	5.7561	7.4709	8.8304	8.8958	5.732	5.9918	5.7752	5.2823	4.8478
138	[87] Ergosterol (RTMS)	331001	(145 + 129), 3311	0.0238	0.0289	0.0238	0.0289	0.0238	5.3888	4.3023	5.1885	5.7561	7.4709	8.8304	8.8958	5.732	5.9918	5.7752	5.2823	4.8478
139	[700] Ergosta-3,7-dien-3-ol	334001	(75), 3348	0.0238	0.0289	0.0238	0.0289	0.0238	5.3888	4.3023	5.1885	5.7561	7.4709	8.8304	8.8958	5.732	5.9918	5.7752	5.2823	4.8478
140	[82] Ergosta-7,22-dien-3-ol (RTMS)	335001	(75), 3348	0.0238	0.0289	0.0238	0.0289	0.0238	5.3888	4.3023	5.1885	5.7561	7.4709	8.8304	8.8958	5.732	5.9918	5.7752	5.2823	4.8478
141	Lanosta-8,24-dien-3-beta-ol	336001	(85 + 129), 3362	0.0238	0.0289	0.0238	0.0289	0.0238	5.3888	4.3023	5.1885	5.7561	7.4709	8.8304	8.8958	5.732	5.9918	5.7752	5.2823	4.8478



Table 6B

ID	METABOLITE	MSTs [MS-ID]	FRAGMENTS [M/Z]_RI	LOADINGS COMPONENT 1	LOADINGS COMPONENT 2	LOADINGS COMPONENT 3	MEOH_AVG	MEOH_RSD	SPIN_AVG	SPIN_RSD	SPINW_AVG	SPINW_RSD	FILTER_AVG	FILTER_RSD
1	[938; Sulfuric acid (2TMS)]	127005		-0,131	0,107	0,04690	54,1	0,28725	44,1	0,00244	0,04384	78,8	17,7	
2	Serine	128001 and 138001	(73 + 227)_1282 (132)_1287 and (218 + 204)_1388			0,63748	47,2	0,08816	157,1	1,02255	17,4	1,52101		
3	Ethanolamine	128002	(174)_1290			0,03898	36,8	0,01582	30,0	0,14660	15,4	0,04714	36,0	
4	Phosphoric acid	129001	(299)_1305			8,67599	26,2	1,94316	83,0	9,53860	24,5	11,41725	23,3	
5	Leucine	129002	(158)_1301	0,107		0,02139	101,0			0,14769	17,2	0,11374	13,5	
6	Glycerol	129003	(218 + 147)_1304	-0,189	0,17	22,51766	29,7	19,22082	11,6	6,67646	20,2	20,87457	36,5	
7	Threonine	132001 and 140001	(130 + 146)_1326 and (219 + 117)_1410			4,06654	22,4	2,12046	39,0	4,39009	13,0	4,42389	16,4	
8	Isoleucine	132002	(158)_1324			0,66056	47,9	0,11210	225,9	1,14786	17,2	1,12338	15,4	
9	Proline	132003	(142 + 216)_1328			2,41173	58,8	0,28813	215,5	5,21658	22,4	5,50778	20,2	
10	Glycine	133001	(174 + 249)_1335			0,32686	28,5	0,25123	24,5	2,76549	23,1	1,10011	21,2	
11	Succinic acid	134001	(129 + 247)_1347			0,22947	17,9	0,25974	18,4	0,09180	22,4	0,13195	23,2	
12	Glyceric acid	135003	(189)_1361			0,05537	16,9	0,06445	20,1	0,02381	26,4	0,02314	18,4	
13	Uracil	136001	(241 + 99)_1370			1,05304	31,0	1,76215	14,7	0,11130	15,9	0,23678	15,0	
14	Fumaric acid	137001	(245)_1380			0,07628	20,1	0,07487	13,6	0,02936	14,5	0,03571	15,7	
15	Alanine	138002	(262 + 188)_1385			0,95528	61,4	0,63123	19,6	0,19579	24,1	2,10684	20,3	
16	[644; 2-Methyl-1,3- butanediol (2TMS)]	140003	(143 + 117)_1401			1,16419	24,6	1,71487	13,0	0,23576	17,5	0,39304	13,5	
17	[700; 2-methyl-1,2- propanediol (2TMS)]	141003	(131 + 73)_1415			1,15500	28,9	1,79539	18,1	0,17400	35,6	0,46504	96,5	
18	[590; 1-Acetyl-2- thiohydantoin]	141004	(158 + 116)_1419			0,28384	37,2	0,17148	31,3	0,11661	38,5	0,13799	23,1	
19	Alanine [BP] (3TMS)	142001	(147 + 160)_1425			0,75654	51,6	0,27925	31,1	0,09809	53,5	0,35573	28,9	
20	[619; 2-(3',4'- Bishydroxyphenyl)-2- oxoethylamine (4TMS)]	143003	(174)_1439			0,00119	32,6		0,06986	24,3	0,00662	58,7		
21	[678; N,N-Di-(2- Hydroxyethyl)- methanamine (2TMS)]	144003	(160)_1444			0,98807	38,7	0,89244	33,1	0,36391	28,7	0,42920	15,6	

22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	144007	(117 + 160)_1452	0,417	-0,36	0,25	0,07329	31,4	0,07453	21,3	0,01119	16,1	0,01407	30,7
		146001	(103 + 218)_1459	0,111			0,07722	144,7	0,05110	43,4	0,37587	15,3	0,41111	16,8
		146003	(147 + 287)_1466				8,95634	26,5	13,17503	11,1	1,08184	12,5	2,40519	16,5
			[709; 2,5-Diaminovalerolactam (2TMS)]				0,03916	292,8	0,01383	24,5	0,86481	9,9	0,43195	41,9
25	Citramalic acid	148001	(247 + 147)_1478				0,74213	12,4	0,67973	15,9	0,46812	11,0	0,50285	11,0
27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	148002	(155)_1482				0,01683	231,6	0,00277	90,7	0,08052	29,0	0,11318	20,3
		149001	(245 + 233)_1490				0,33171	15,3	0,29746	11,1	0,13024	6,8	0,15265	16,6
		150002	(117 + 103)_1504				0,12467	13,6	0,14850	9,6	0,06331	12,4	0,07366	12,2
		150003	(128 + 305)_1496				2,42808	76,2	1,18180	94,1	8,00131	13,3	6,63323	14,1
31	[622; Parabanic acid (2TMS)]	151002	(115 + 100)_1507				0,04023	62,0	0,02184	48,8	0,07220	26,9	0,07372	27,2
32	[729; N,N-Dimethyllysine methyl ester]	151003	(188)_1514			0,225	0,03363	80,0	0,00561	82,4	0,18647	26,4	0,17987	28,3
		152001	(128 + 176)_1523			0,103	0,11030	77,8	0,07052	84,5	0,34268	14,9	0,29565	19,2
		152002	(232 + 73)_1521				3,76798	67,2	3,07925	83,0	9,38512	31,3	8,04427	18,0
		153002	(258 + 156)_1530				26,15039	11,7	20,48811	11,5	5,15064	14,8	15,62416	25,1
36	[596; N-Acetylglutamic acid (2TMS)]	154002	(84 + 158)_1539				4,21470	45,7	0,80105	48,3	4,24163	24,9	4,67381	22,9
		157001 and 164001	(146 + 120)_1563 and (192 + 218)_1641				1,43566	26,1	0,84550	22,6	1,94035	13,6	1,49406	13,5
38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	157002	(265 + 191)_1577				0,26500	16,1	0,27966	8,1	0,07596	14,5	0,09925	14,5
		158002	(179)_1581				1,33862	35,6	1,90258	15,8	0,04643	30,2	0,11231	42,6
40	[639; Proline (2TMS)]	158003	(275 + 377)_1582	0,288	-0,222		8,40360	11,9	6,91488	8,4	4,69522	6,4	5,30098	10,9
		159001	(186 + 142)_1595				0,86547	57,7	0,33766	21,8	0,22407	73,3	0,44558	38,9
		163001	(348 + 246)_1631				2,10220	91,6	0,20774	111,4	12,83440	7,0	7,71483	19,1
		165002	(73 + 200)_1652				0,10092	123,5	0,14523	36,0	0,16876	12,6	0,28035	59,4
44	[910; 2-Ketogluconic acid (2TMS)]	166002	(204 + 73)_1660				0,78390	50,0	0,17132	23,9	0,00653	24,4	0,04955	52,1

45	acid methoxyamine (4TMS)]	167001	(128)_1675	0,00543	63,2	0,00806	40,6	0,01589	31,4	0,01259	30,0
46	Homocysteine	167002	(217 + 103)_1671	0,113	0,13	2,28653	9,0	0,01760	30,7	0,17752	25,1
47	Arabinose	167003	(288 + 98)_1673			0,04381	34,0	0,43587	24,6	0,15631	124,4
48	[NA]	168001	(188 + 116)_1683	-0,184	0,294	0,05239	71,4	0,05239	22,7	0,84501	24,5
49	Asparagine										
50	[877; Pyrophosphoric acid (4TMS)]	168004	(451)_1676			0,00297	51,5	0,05781	247,2	0,13630	148,3
51	[746; Ribonic acid-1,4- lactone (3TMS)]	169001	(117 + 204)_1695			0,02106	27,3	0,02977	10,8	0,00544	28,7
52	[499; 2-Ethyl-3- hydroxy-3- methylvaleric acid (2TMS)]	171003	(275)_1708			0,00436	81,5	0,00177	62,6	0,02153	29,1
53	[NA]	172005	(173)_1721			0,00234	48,5	0,00986	13,9	0,12867	17,2
54	Glycerol-2-phosphate	174002	(243 + 211)_1736			0,03175	45,0	0,04793	16,3	0,04808	37,5
55	[NA]	174003	(205 + 200)_1742			0,06785	26,4	0,15545	22,4	0,00404	45,1
56	[612; 4-Aminobutyric acid (2TBS)]	175003	(112)_1748			0,00203	39,9	0,00121	0,03810	26,8	0,00295
57	[829; Orotic acid (3TMS)]	176003	(254 + 191)_1756			0,18805	24,6	0,31013	21,4	0,00900	20,9
58	[757; 2-Desoxy-pentos- 3-ylose dimethoxyamine (2TMS)]	176004	(231)_1762			0,54042	30,3	1,00311	13,5	0,00447	38,7
59	[636; 4R-Acetamido- 2,3-(Z)-epoxy-4-(E)- hydroxycyclohexane (1TMS)]	176005	(258 + 184)_1756			0,66810	25,0	0,18438	57,6	0,55413	26,0
60	Ornithine; Arginine	176006 and 182002	(348 + 174)_1765 and (174 + 142)_1821			12,71146	36,2	6,18480	54,1	25,49810	5,7
61	Glycerol-3-phosphate	177002	(357 + 299)_1770			1,51001	37,9	0,55731	18,7	1,93909	21,1
62	[NA]	177003	(172 + 199)_1772			0,08711	19,3	0,10294	22,4	0,18897	28,8
63	[812; D-Xylofuranose (4TMS)]	177004	(217)_1775			0,59196	9,5	0,66360	17,1	0,22017	21,9
64	Glutamine	178001	(157 + 155)_1782			0,01596	37,0	0,02963	11,4	0,88746	28,9
65	[789; Tyramine (3TMS)]	179002	(174)_1795			0,09827	15,9	0,08696	14,8	0,06782	23,1
66	[646; 3-Deoxyglucitol (5TMS)]	180001	(147 + 231)_1798			0,29976	27,3	0,45993	10,0	0,00558	25,1
67	Glyceric acid-3- phosphate	181003	(211 + 299)_1814			0,08052	18,8	0,04123	19,1	0,09475	13,3

67	Citric acid [570; Hypoxanthine (2TMS)]	182004	(273 + 133)_1823	1,69956	11,0	1,12285	15,0	2,09056	6,3	1,49388	12,5
68	Arginine [693; 2-Furan-2- hydroxyacetic acid (2TMS)]	182006	(265)_1825	0,00142	71,5	0,00200	71,9	0,01528	21,0		
69	Arginine [731; Erythrose (3TMS)]	183001	(157 + 256)_1830	0,47655	143,9	0,14081	21,6	3,97138	33,8	2,24025	39,3
70	Glucose [919; D-Xylopyranose (4TMS)]	184002	(169)_1842	1,57428	25,9	1,50269	48,3	0,26648	43,5	1,03882	21,3
71	Glucose [708; Glucose methoxyamine (5TMS)]	184003	(226 + 217)_1836	0,43193	13,0	0,23600	22,5	0,36580	12,8	0,30404	12,6
72	Glucose [912; Tetradecanoic acid (1TMS)]	184004	(191 + 204)_1843	0,04721	50,8	0,12192	128,7	0,14119	114,9	0,11616	67,6
73	Lysine [826; beta-[[[5-methyl- 2- thienyl)methyl]eneamino -benzeneacetic acid methyl ester]	185003	(217)_1849	0,32464	48,8	0,19307	141,5	0,01543	38,6	0,06350	31,8
74	Fructose [772; D-Glucose (5TMS)]	185004	(132 + 285)_1853	0,59460	49,6	0,08803	49,6	0,04033	32,9	0,03144	36,4
75	Fructose [793; D-Galactono-1,4- lactone (4TMS)]	186002	(200 + 174)_1858	14,76856	19,7	4,45895	50,3	14,88358	29,8	20,84967	10,8
76	Fructose [945; beta-D- Glucopyranose (5TMS)]	187002 and 188004	(217 + 104)_1868 and (307 + 217)_1878	-0,227 0,28							
77	Glucose [775; Dopamine (4TMS)]	187004	(241 + 153)_1871	6,67832	19,7	3,48593	28,9	0,14513	12,6	1,58925	23,5
78	Glucose [793; D-Galactono-1,4- lactone (4TMS)]	187004	(241 + 153)_1871	2,74057	79,2	0,33047	101,7	15,42558	12,6	4,73391	41,9
79	Glucose [793; D-Galactono-1,4- lactone (4TMS)]	188002	(205 + 160)_1883	0,24653	34,1	0,15541	78,9	0,01229	49,0	0,05665	48,4
80	Glucose [793; D-Galactono-1,4- lactone (4TMS)]	189002 and 191001	(160 + 186)_1893 and (205 + 217)_1913	11,81490	24,1	6,15313	25,1	1,26687	49,6	15,42455	15,2
81	Glucose [793; D-Galactono-1,4- lactone (4TMS)]	189005	(191 + 204)_1889	6,38932	48,7	7,97918	53,2	0,55170	109,6	9,45443	62,7
83	Glucose [793; D-Galactono-1,4- lactone (4TMS)]	189006 and 194002	(179)_1893 and (218 + 73)_1941	4,00024	32,8	0,74048	27,5	30,75162	22,4	6,25730	21,4
84	Glucose [793; D-Galactono-1,4- lactone (4TMS)]	193001	(217 + 319)_1932	2,05659	12,2	0,24987	59,9	1,20994	14,2	1,38047	13,8
85	Glucose [793; D-Galactono-1,4- lactone (4TMS)]	193002	(205 + 73)_1925	1,34133	40,8	39,64590	10,8	2,84657	42,6	1,10745	16,9
86	Glucose [793; D-Galactono-1,4- lactone (4TMS)]	192007	(287)_1921	0,14313	18,8			0,08837	19,1	0,08248	13,7
87	Glucose [793; D-Galactono-1,4- lactone (4TMS)]	196004	(217 + 361)_1957	3,45775	37,1	4,75847	24,7	0,01175	51,5	0,33227	27,6
88	Glucose [793; D-Galactono-1,4- lactone (4TMS)]	197002	(204 + 191)_1974	14,06842	40,1	18,23390	15,5	0,82313	114,7	12,74981	60,2
89	Glucose [793; D-Galactono-1,4- lactone (4TMS)]	200001	(147 + 217)_2001	0,45174	13,4	0,98323	26,6	0,05023	35,0	0,12700	23,7
89	Glucose [793; D-Galactono-1,4- lactone (4TMS)]	200002	(174 + 175)_2005	0,00291	27,5	0,01220	52,8	0,40778	22,5	0,00347	17,6

90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	203002	(96 + 311)_2030	0,12643	25,4	0,19866	46,9	0,22671	41,8	0,09010	44,9
91	[766; beta-D-Methylglucopyranoside (4TMS)]	203003	(158 + 204)_2024	0,17110	192,9	5,39073	66,6	0,02556	46,1	0,13795	84,7
92	[680; Glycerol-2-phosphate (4TMS)]	203004	(243 + 299)_2026	0,14684	15,8	0,22620	27,9	0,00426	25,5	0,09477	23,5
93	[607; Putrescine (4TMS)]	204003	(174 + 214)_2041	0,01457	41,3	0,15329	143,4	0,02308	16,0	0,00973	50,4
94	[770; 3,4,6-Trisubstituted Hexadecanoic acid (4TMS)]	205001	(132 + 313)_2049	5,75408	42,1	0,54067	39,3	0,91947	34,5	0,43968	25,7
95	[756; beta-D-Trisubstituted phenylethanolamine (5TMS)]	206001	(174)_2065	0,00295	61,3	0,00907	82,3	0,03216	18,0	0,00799	43,3
96	[697; Ribose-5-phosphate (4TMS)]	209002	(305)_2092	0,01091	31,3	0,00976	19,0	0,00804	13,5	0,01034	81,8
97	[756; beta-D-Methylglucopyranoside (4TMS)]	209004	(204 + 73)_2088	0,76284	126,8	10,96125	60,4	0,00674	58,7	0,28192	44,5
98	[662; Ribose-5-phosphate (5TMS)]	211003	(315)_2113	0,00249	65,8	0,00460	49,9	0,02693	20,5	0,03134	26,6
99	[857; Mannitol (5TMS)]	211004	(315 + 217)_2109	0,05099	24,9	0,12094	18,0	0,00601	30,1	0,00403	15,0
100	[832; Dopamine (4TMS)]	213001	(73 + 319)_2132	0,30723	9,4	0,26158	19,3	0,14686	30,5	0,12892	31,0
101	[904; Galactose (5TMS)]	213003	(174 + 73)_2126	0,22364	126,6	0,99691	67,4	0,04041	28,2	0,09739	25,2
102	[648; Ethylamine (5TMS)]	214003	(103 + 319)_2138	0,10823	15,5	0,09096	15,8	0,06025	32,5	0,05652	28,0
103	[795; Erythritol (4TMS)]	216002	(174 + 73)_2163	0,51105	119,9	2,09798	55,0	0,02789	27,1	0,08845	57,9
104	[705; 2-Ketogluconic acid (5TMS)]	216003	(73 + 217)_2156	0,34387	57,2	0,08694	44,0	0,04710	37,5	0,14213	15,3
105	[733; Threitol (4TMS)]	217002	(73)_2169	0,33596	101,9	1,31509	51,8			0,03460	40,7
106	[9-(Z)-Octadecenoic acid (5TMS)]	218001	(73 + 103)_2181	0,87458	52,5	0,26366	22,5	0,02928	24,8	0,10677	25,6
107	[129 + 117)_2225 Octadecenoic acid (5TMS)]	222001	(75 + 117)_2218	0,43809	21,1	0,46713	44,3	0,73988	38,5	0,31844	23,1
108	[341 + 117)_2247 Octadecanoic acid (5TMS)]	223003	(129 + 117)_2225	0,06612	32,1	0,06216	54,6	0,13655	46,7	0,07367	33,4
109	[715; Erythritol (4TMS)]	225002	(341 + 117)_2247	13,43152	35,2	0,34054	44,1	0,50376	35,9	0,28095	18,1
110	[217 + 84)_2259 Octadecanoic acid (5TMS)]	226001	(217 + 84)_2259	0,39538	44,0	0,08569	25,5	0,00353	33,4	0,02350	41,3

111	[583; Erythritol (4TMS)]	228001	(290)_2284	0,00884	32,3	0,00661	25,0	0,00596	37,5	0,00603	30,0
	[877; beta-D- Galactopyranoside- 1,2-glycerol (6TMS)]	230001	(204)_2296	0,02126	20,0	0,01971	11,6	0,01436	12,3	0,01394	16,8
113	Galactose-6-phosphate	232001	(387 + 160)_2315	0,16933	18,7	0,07902	11,3	0,01624	41,4	0,09292	26,2
114	Fructose-6-phosphate	232002	(315)_2314	0,13866	31,7	0,05854	12,9	0,01596	36,6	0,07726	21,1
115	Glucose-6-phosphate 233002 and (387 + 73)_2350	235002	(73 + 387)_2330 and (387 + 73)_2350	4,37575	16,8	2,57163	11,1	0,39383	26,0	1,77442	23,3
	[882; Pseudouridine (5TMS)]	234001	(218 + 217)_2346	0,14296	38,7			0,07201	47,3	0,00214	27,2
117	[724; Glycerol (3TMS)]	238002	(103 + 73)_2385	0,37948	40,6	0,10653	26,3	0,02356	32,8	0,03491	30,5
118	[928; Glucopyranose-6- phosphate (6TMS)]	239001	(204 + 73)_2393	0,10559	68,7	0,08408	77,5	0,04797	133,6	0,16396	78,1
	[931; myo-Inositol-2- phosphate (7TMS)]	243001	(299 + 318)_2431	0,18509	37,4	0,15458	62,1	0,31648	39,3	0,05333	27,7
120	[945; Uridine (3TMS)]	248002	( 73)_2480	0,48761	53,4	0,50953	28,6	0,23973	9,7	0,27644	14,1
121	[657; Erythritol (4TMS)]	249001	(217 + 103)_2493	0,10447	47,8	0,02791	25,7	0,00710	25,0	0,01428	31,7
	[644; Erythritol (4TMS)]	252002	(446 + 156)_2519	0,15058	49,4	0,04070	28,5	0,00193	9,3	0,00634	38,5
123	[945; Galactofuranose- 6-phosphate (7TMS)]	256001	(387 + 73)_2565	0,44993	18,4	0,21054	11,6	0,13306	25,4	0,36436	18,5
	[734; 1- Monooleoylglycerol (2TMS); 1- Monohexadecenylglyc erol (1TMS)]	258001	(129)_2583	0,00841	18,4	0,00477	51,4	0,01023	48,5	0,00562	49,4
124	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta- D-Fru]	262001	(361 + 73)_2620	9,53198	32,8	9,04470	34,8	0,33110	11,7	6,96516	33,8
126	[559; Erythritol (4TMS)]	266001	(73 + 127)_2657	-0,169	46,5	0,05594	27,3			0,02097	21,0
	[777; Fructose-6- phosphate methoxyamine (6TMS)]	272001	(387 + 315)_2726	0,14843	31,5	0,15099	24,7			0,04015	51,0
128	[824; D-Sedoheptulose- 7-phosphate (7TMS)]	272002	(73 + 315)_2721	0,28926	45,2	0,37903	37,5	0,00448		0,06549	61,4
	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D- Glc]	273002	(204 + 160)_2734	0,28811	28,2	0,54840	11,0	0,00902	28,7	0,05010	87,9

130	Trehalose [626; 5-Methylthioadenosine [3TMS]]	274002	(183 + 169)_2747	3,69549	24,5	2,56889	23,4	4,08567	47,6	4,63159	27,5
131	[895; Isomaltose methoxyamine (8TMS)]	277004	(164)_2770	0,00664	62,3	0,01537	26,6	0,04186	21,0	0,01935	18,1
132	[855; Squalene]	281001	(204)_2817	0,08980	41,0	0,07507	20,6	0,00106	6,7	0,00215	41,7
133	Isomaltose	283001	(94 + 81)_2830	0,25946	30,7	0,09586	78,7	0,13483	86,4	0,13584	56,2
134	[902; Melibiose (8TMS); alpha-D-Gal- (1,6)-D-Glc (8TMS)]	287001 and 291002	(361 + 73)_2872 and (73 + 361)_2908	4,75941	27,1	8,64396	7,1	0,09182	24,1	0,56071	21,8
135	[748; D-Sedoheptulose- 7-phosphate (7TMS)]	293001	(204)_2932	0,40738	17,0	0,36285	11,1	0,30764	9,1	0,27061	11,3
136	Ergosterol	318001	(315 + 73)_3188	0,16723	57,5	0,09328	77,1				
137	[674; Ergosterol (1TMS)]	327001	(337 + 81)_3270	0,73100	29,0	0,26381	78,5	0,66772	46,1	0,17283	32,5
138	[700; Ergosta-5,7-dien- 3-ol]	331001	(145 + 129)_3311	0,03285	47,0	0,00815	46,1	0,01514	55,5	0,00844	24,4
139	[692; Ergosta-7,22-dien- 3-ol (1TMS)]	334001	(75)_3338	0,00913	39,3	0,00794	41,9	0,01095	57,1	0,00307	1,1
140	Lanosta-8,24-dien-3- beta-ol	335001	(75)_3349	0,02242	25,2	0,01520	28,1	0,01799	43,5	0,00804	30,0
141		338001	(95 + 129)_3382	0,05562	28,0	0,02548	57,1	0,04597	52,3	0,01179	36,5

1st ID	1st METABOLITE	2nd ID	2nd METABOLITE	NUMBER OF PAIRS	KENDALL'S CORRELATION	PEARSON'S CORRELATION	EUCLIDIAN DISTANCE	MUTUAL INFORMATION	RANK: POSITIVE KENDALL'S CORRELATION	RANK: NEGATIVE KENDALL'S CORRELATION	RANK: POSITIVE PEARSON'S CORRELATION	RANK: NEGATIVE PEARSON'S CORRELATION	RANK: EUCLIDIAN DISTANCE	RANK: MUTUAL INFORMATION	DUPPLICATE/ORIGINAL
53	1 [938; Sulfuric acid (2TM	54 [NA]		36	0.616	0.754	5.037	0.592	1	140	5	136	2	32	original
128	1 [938; Sulfuric acid (2TM	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]		36	0.597	0.720	9.158	0.621	2	139	7	134	29	16	original
46	1 [938; Sulfuric acid (2TM	47 [NA]		36	0.584	0.786	5.549	0.662	3	138	2	139	3	4	original
45	1 [938; Sulfuric acid (2TM	48 Arabinose		36	0.575	0.692	16.915	0.649	4	137	8	133	96	6	original
56	1 [938; Sulfuric acid (2TM	57 [757; 2-Desoxy-pentos-3-yose dimethoxyamine (2TMS)]		35	0.570	0.560	12.242	0.629	5	136	27	114	65	12	original
12	1 [938; Sulfuric acid (2TM	13 Uracil		36	0.549	0.686	16.330	0.605	6	135	9	132	95	21	original
64	1 [938; Sulfuric acid (2TM	65 [846; 3-Deoxyglucitol (5TMS)]		36	0.546	0.606	9.256	0.651	7	134	19	122	31	5	original
15	1 [938; Sulfuric acid (2TM	16 [844; 2-Methyl-1,3-butanediol (2TMS)]		36	0.533	0.660	17.033	0.588	8	133	13	128	99	35	original
83	1 [938; Sulfuric acid (2TM	84 Mannitol		34	0.533	0.769	25.565	0.584	9	132	3	138	130	37	original
49	1 [938; Sulfuric acid (2TM	50 [746; Ribonic acid-1,4-lactone (3TMS)]		36	0.527	0.673	10.184	0.587	10	131	10	131	41	36	original
23	1 [938; Sulfuric acid (2TM	24 [725; 2-Ketocacetic acid (2TMS)]		36	0.524	0.657	28.542	0.601	11	130	14	127	134	23	original
16	1 [938; Sulfuric acid (2TM	17 [700; 2-methyl-1,2-propanediol (2TMS)]		36	0.514	0.648	16.990	0.600	12	129	15	126	98	26	original
98	1 [938; Sulfuric acid (2TM	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]		34	0.512	0.806	4.952	0.590	13	128	1	140	1	33	original
133	1 [938; Sulfuric acid (2TM	134 Isomaltose		36	0.502	0.666	24.656	0.614	14	127	12	129	128	18	original
55	1 [938; Sulfuric acid (2TM	56 [829; Gluconic acid		36	0.495	0.670	7.459	0.639	15	126	17	124	71	31	original
87	1 [938; Sulfuric acid (2TM	88 Gluconic acid		36	0.479	0.607	12.254	0.548	16	125	11	130	15	9	original
62	1 [938; Sulfuric acid (2TM	63 Glutamine		35	0.455	0.057	12.254	0.548	17	124	56	85	66	53	original
90	1 [938; Sulfuric acid (2TM	91 [766; beta-D-Methylglucopyranoside (4TMS)]		36	0.438	0.723	13.771	0.471	18	123	6	135	82	77	original
96	1 [938; Sulfuric acid (2TM	97 [756; beta-D-Methylglucopyranoside (4TMS)]		36	0.422	0.762	18.847	0.597	19	122	4	137	111	30	original
61	1 [938; Sulfuric acid (2TM	62 [812; D-Xylofuranose (4TMS)]		36	0.419	0.580	13.364	0.599	20	121	24	117	78	27	original
38	1 [938; Sulfuric acid (2TM	39 [829; 1-Phenylethanol (1TMS)]		36	0.413	0.558	16.923	0.589	21	120	28	113	97	34	original
28	1 [938; Sulfuric acid (2TM	29 Erythritol		36	0.397	0.570	7.259	0.604	22	119	25	116	13	22	original
10	1 [938; Sulfuric acid (2TM	11 Succinic acid		36	0.371	0.462	9.033	0.574	23	117	31	110	28	43	original
71	1 [938; Sulfuric acid (2TM	72 [919; D-Xylopyranose (4TMS)]		35	0.371	0.450	6.839	0.444	24	118	34	107	8	86	original
100	1 [938; Sulfuric acid (2TM	101 [832; Dopamine (4TMS)]		36	0.365	0.588	9.941	0.361	25	116	21	120	38	112	original
104	1 [938; Sulfuric acid (2TM	102 [705; 2-Ketogluconic acid (5TMS)]		35	0.351	0.598	10.884	0.481	26	115	20	121	52	70	original
11	1 [938; Sulfuric acid (2TM	12 Glycine		36	0.349	0.466	7.392	0.538	27	114	30	111	14	58	original
85	1 [938; Sulfuric acid (2TM	86 [793; D-Galactono-1,4-lactone (4TMS)]		33	0.348	0.585	21.093	0.619	28	113	23	118	116	17	original
102	1 [938; Sulfuric acid (2TM	103 [848; Ethylamine (2TMS)]		36	0.343	0.585	13.393	0.475	29	112	22	119	81	74	original
91	1 [938; Sulfuric acid (2TM	92 [860; Glycerol-2-phosphate (4TMS)]		36	0.340	0.608	6.996	0.558	30	111	18	123	9	50	original



86	1 [938; Sulfuric acid (2TM. 87 [945; beta-D-Glucopyranose (5TMS)]	34	0.337	0.633	30.342	0.628	31	110	16	125	138	13 original
52	1 [938; Sulfuric acid (2TM. 53 Glycerol-2-phosphate	36	0.327	0.494	8.404	0.377	32	108	29	112	22	107 original
92	1 [938; Sulfuric acid (2TM. 93 [607; Putrescine (4TMS)]	34	0.305	0.423	10.064	0.335	33	108	37	104	40	122 original
51	1 [938; Sulfuric acid (2TM. 52 [NA]	25	0.273	0.151	16.234	0.583	34	107	50	91	94	38 original
89	1 [938; Sulfuric acid (2TM. 90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	36	0.232	0.338	7.897	0.355	35	108	39	102	17	113 original
130	1 [938; Sulfuric acid (2TM. 131 [626; 5-Methylthioadenosine (3TMS)]	29	0.222	0.146	13.390	0.449	36	105	51	90	80	84 original
88	1 [938; Sulfuric acid (2TM. 89 [775; Dopamine (4TMS)]	16	0.217	-0.290	12.156	0.387	37	104	90	51	64	105 original
48	1 [938; Sulfuric acid (2TM. 49 [877; Pyrophosphoric acid (4TMS)]	36	0.206	0.208	17.136	0.472	38	103	47	94	100	76 original
124	1 [938; Sulfuric acid (2TM. 125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	36	0.190	0.460	27.807	0.575	39	102	32	108	133	42 original
37	1 [938; Sulfuric acid (2TM. 38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	36	0.187	0.436	9.345	0.614	40	101	36	105	33	19 original
69	1 [938; Sulfuric acid (2TM. 70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	30	0.182	0.039	17.716	0.463	41	100	60	81	104	79 original
119	1 [938; Sulfuric acid (2TM. 120 [945; Uridine (3TMS)]	33	0.167	0.241	11.844	0.534	42	99	43	98	60	62 original
60	1 [938; Sulfuric acid (2TM. 61 [NA]	36	0.165	-0.050	8.084	0.426	43	98	71	70	19	97 original
24	1 [938; Sulfuric acid (2TM. 25 [709; 2,5-Diaminovalerolactam (2TMS)]	35	0.150	-0.425	15.768	0.541	44	97	101	40	91	56 original
42	1 [938; Sulfuric acid (2TM. 43 [548; Leucine (2TBS)]	32	0.141	0.047	8.377	0.351	45	96	59	82	21	116 original
13	1 [938; Sulfuric acid (2TM. 14 Fumaric acid	36	0.127	0.367	7.238	0.523	46	95	38	103	12	63 original
21	1 [938; Sulfuric acid (2TM. 22 [690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	30	0.122	0.455	6.806	0.579	47	94	33	108	7	40 original
20	1 [938; Sulfuric acid (2TM. 21 [878; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	36	0.117	0.282	15.344	0.429	48	93	40	101	90	94 original
127	1 [938; Sulfuric acid (2TM. 128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	33	0.102	0.219	9.318	0.557	49	92	45	96	32	52 original
79	1 [938; Sulfuric acid (2TM. 80 [772; D-Glucose (5TMS)]	34	0.080	0.446	25.126	0.558	50	91	35	108	129	51 original
97	1 [938; Sulfuric acid (2TM. 98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	23	0.075	-0.198	17.365	0.334	51	90	79	62	102	124 original
111	1 [938; Sulfuric acid (2TM. 112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	35	0.069	0.141	11.472	0.427	52	89	53	88	57	96 original
131	1 [938; Sulfuric acid (2TM. 132 [895; Isomaltose methoxyamine (8TMS)]	32	0.056	0.565	6.661	0.567	53	88	26	115	6	47 original
115	1 [938; Sulfuric acid (2TM. 116 [882; Pseudouridine (5TMS)]	17	0.044	0.280	6.580	0.534	54	87	41	100	5	61 original
44	1 [938; Sulfuric acid (2TM. 45 Homocysteine	33	0.034	0.032	17.233	0.418	55	86	61	80	101	100 original
95	1 [938; Sulfuric acid (2TM. 96 myo-Inositol	26	0.034	0.217	10.733	0.335	56	85	46	95	50	121 original
25	1 [938; Sulfuric acid (2TM. 26 Citramalic acid	36	0.025	0.169	14.651	0.477	57	84	48	93	87	71 original
106	1 [938; Sulfuric acid (2TM. 107 9-(Z)-Octadecenoic acid	36	0.013	-0.028	12.819	0.351	58	83	69	72	72	117 original
22	1 [938; Sulfuric acid (2TM. 23 Homoserine	36	0.003	0.281	10.572	0.428	59	82	89	52	48	95 original
128	1 [938; Sulfuric acid (2TM. 127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	33	-0.011	0.121	7.073	0.520	60	81	54	87	10	64 original
81	1 [938; Sulfuric acid (2TM. 82 Lysine	17	-0.015	-0.457	8.644	0.470	61	80	104	37	24	78 original
84	1 [938; Sulfuric acid (2TM. 85 [528; Methylcitric acid (4TMS)]	20	-0.021	0.220	7.135	0.430	62	79	44	97	11	92 original
5	1 [938; Sulfuric acid (2TM. 6 Glycerol	36	-0.022	0.087	33.664	0.568	63	78	55	86	139	45 original
134	1 [938; Sulfuric acid (2TM. 135 [902; Melibiose (8TMS); alpha-D-Gal(1,6)-D-Glc (8TMS)]	36	-0.028	0.013	11.727	0.334	64	77	64	77	58	123 original
27	1 [938; Sulfuric acid (2TM. 28 Malic acid	36	-0.048	0.277	10.364	0.498	65	76	42	99	44	66 original
4	1 [938; Sulfuric acid (2TM. 5 Leucine	18	-0.059	-0.297	8.154	0.162	66	75	91	50	20	139 original
118	1 [938; Sulfuric acid (2TM. 119 [931; myo-Inositol-2-phosphate (7TMS)]	36	-0.060	-0.016	8.928	0.389	67	73	68	73	26	104 original
107	1 [938; Sulfuric acid (2TM. 108 Octadecenoic acid	36	-0.060	-0.232	9.210	0.391	68	74	85	56	30	102 original
101	1 [938; Sulfuric acid (2TM. 102 [904; Galactose methoxyamine (5TMS)]	36	-0.063	0.006	7.831	0.542	69	72	85	76	16	55 original
47	1 [938; Sulfuric acid (2TM. 48 Asparagine	36	-0.098	-0.384	10.912	0.568	70	71	97	44	63	46 original
138	1 [938; Sulfuric acid (2TM. 139 [700; Ergosta-5,7-dien-3-ol]	25	-0.120	-0.040	13.035	0.288	71	70	70	71	73	128 original
77	1 [938; Sulfuric acid (2TM. 78 Mannose	35	-0.123	-0.003	9.559	0.560	72	69	67	74	35	48 original
139	1 [938; Sulfuric acid (2TM. 140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	28	-0.132	0.056	9.966	0.327	73	68	57	84	39	126 original
135	1 [938; Sulfuric acid (2TM. 136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.132	-0.342	6.088	0.351	74	67	92	49	4	118 original
72	1 [938; Sulfuric acid (2TM. 73 [708; Glucose methoxyamine (5TMS)]	29	-0.138	-0.090	11.380	0.453	75	66	112	29	61	140 original
67	1 [938; Sulfuric acid (2TM. 68 [570; Hypoxanthine (2TMS)]	8	-0.143	-0.054	10.899	-0.047	76	65	72	69	45	81 original
17	1 [938; Sulfuric acid (2TM. 18 [590; 1-Acetyl-2-thiohydantoin]	36	-0.152	-0.135	9.849	0.435	77	64	74	67	36	91 original
39	1 [938; Sulfuric acid (2TM. 40 [880; 2,3-Dimethylsuccinic acid (2TMS)]	36	-0.162	0.016	27.855	0.545	78	63	63	78	132	54 original
110	1 [938; Sulfuric acid (2TM. 111 [583; Erythritol (4TMS)]	29	-0.167	-0.145	14.484	0.369	79	62	75	68	85	111 original
99	1 [938; Sulfuric acid (2TM. 100 [857; Mannitol (6TMS)]	36	-0.168	0.051	10.263	0.600	80	60	58	83	42	24 original



66	1	[938; Sulfuric acid (2TM	67	Citric acid	36	-0,540	-0,718	18,993	0,375	130	11	130	11	112	108 original
2	1	[938; Sulfuric acid (2TM	3	Ethanolamine	34	-0,547	-0,813	12,364	0,598	131	10	139	2	89	29 original
59	1	[938; Sulfuric acid (2TM	60	Glycerol-3-phosphate	36	-0,549	-0,734	17,629	0,534	132	9	132	9	103	60 original
57	1	[938; Sulfuric acid (2TM	58	[636; 4R-Acetalamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	36	-0,552	-0,619	15,175	0,371	133	8	116	25	89	109 original
80	1	[938; Sulfuric acid (2TM	81	Tyrosine	36	-0,556	-0,862	23,205	0,623	134	7	140	1	122	15 original
65	1	[938; Sulfuric acid (2TM	66	Glyceralic acid-3-phosphate	36	-0,559	-0,808	9,851	0,569	135	6	138	3	37	44 original
8	1	[938; Sulfuric acid (2TM	9	Proline	35	-0,563	-0,769	22,193	0,342	136	5	136	5	119	119 original
6	1	[938; Sulfuric acid (2TM	7	Threonine	36	-0,568	-0,699	23,486	0,284	137	4	127	14	124	129 original
19	1	[938; Sulfuric acid (2TM	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	8	-0,571	-0,770	9,388	0,223	138	3	137	4	34	136 original
35	1	[938; Sulfuric acid (2TM	36	[596; N-Acetylglutamic acid (2TMS)]	36	-0,587	-0,747	22,300	0,417	139	2	133	8	120	89 original
7	1	[938; Sulfuric acid (2TM	8	Isoleucine	27	-0,601	-0,755	17,862	0,264	140	1	134	7	105	131 original
147	2	Serine	9	Proline	61	0,809	0,965	10,969	0,599	1	140	1	140	6	2 original
146	2	Serine	8	Isoleucine	55	0,700	0,930	5,391	0,558	2	139	2	139	1	11 original
169	2	Serine	31	[622; Parabenic acid (2TMS)]	62	0,662	0,743	20,694	0,463	3	138	15	126	69	43 original
170	2	Serine	32	[728; N,N-Dimethyllysine methyl ester]	62	0,660	0,852	19,023	0,542	4	137	5	138	58	17 original
208	2	Serine	68	[570; Hypoxanthine (2TMS)]	19	0,849	0,682	19,453	0,499	5	136	21	120	59	26 original
171	2	Serine	33	Methionine	62	0,626	0,686	13,188	0,469	6	135	20	121	10	41 original
161	2	Serine	23	Homoserine	62	0,625	0,603	13,919	0,491	7	134	29	112	13	27 original
204	2	Serine	68	Glyceralic acid-3-phosphate	62	0,821	0,770	17,662	0,487	8	133	12	129	44	30 original
165	2	Serine	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	0,818	0,670	25,409	0,524	9	132	22	119	98	21 original
168	2	Serine	30	[815; Ethyl-3-(2H)-thiophenone]	62	0,815	0,759	17,927	0,543	10	131	14	127	48	16 original
145	2	Serine	7	Threonine	62	0,802	0,868	20,208	0,551	11	130	4	137	65	15 original
213	2	Serine	75	Lysine	62	0,570	0,875	28,104	0,552	12	129	3	138	123	13 original
197	2	Serine	59	Ornithine; Arginine	62	0,545	0,829	29,417	0,539	13	127	6	135	130	18 original
172	2	Serine	34	Aspartic acid	62	0,545	0,644	21,962	0,482	14	128	23	118	81	34 original
196	2	Serine	58	[636; 4R-Acetalamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	62	0,537	0,827	9,857	0,532	15	126	7	134	4	19 original
236	2	Serine	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	47	0,530	0,543	26,575	0,483	16	125	33	108	117	33 original
219	2	Serine	81	Tyrosine	62	0,515	0,731	21,597	0,555	17	124	16	125	77	12 original
180	2	Serine	42	Glutamic acid	60	0,506	0,824	14,823	0,552	18	123	8	133	21	14 original
207	2	Serine	69	Arginine	60	0,489	0,695	9,927	0,515	19	122	19	122	5	22 original
175	2	Serine	37	Phenylalanine	62	0,479	0,780	14,786	0,527	20	121	11	130	19	20 original
215	2	Serine	77	[826; beta-[[[5-methyl-2-thienyl)methyl]amino]-benzeneacetic acid methyl ester]	61	0,477	0,822	16,328	0,570	21	120	9	132	31	8 original
148	2	Serine	10	Glycine	62	0,469	0,615	11,572	0,440	22	119	27	114	8	59 original
141	2	Serine	3	Ethanolamine	61	0,416	0,639	20,493	0,472	23	118	24	117	68	39 original
183	2	Serine	45	Homocysteine	59	0,402	0,298	32,235	0,445	24	117	43	98	138	54 original
143	2	Serine	5	Leucine	45	0,396	0,803	19,635	0,640	25	116	10	131	60	1 original
189	2	Serine	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	0,351	0,707	30,606	0,573	26	115	18	123	133	7 original
183	2	Serine	25	[709; 2,5-Diaminovalerolactam (2TMS)]	46	0,329	0,576	17,445	0,385	27	114	31	110	40	97 original
181	2	Serine	43	[548; Leucine (2TBS)]	59	0,324	0,242	15,776	0,389	28	113	44	97	24	84 original
274	2	Serine	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0,324	0,554	6,442	0,263	29	112	32	109	2	136 original
186	2	Serine	48	Asparagine	62	0,310	0,404	16,290	0,437	30	111	38	103	30	61 original
174	2	Serine	36	[596; N-Acetylglutamic acid (2TMS)]	62	0,302	0,709	17,808	0,513	31	110	17	124	46	23 original
188	2	Serine	60	Glycerol-3-phosphate	62	0,298	0,619	14,012	0,503	32	108	25	116	14	25 original
205	2	Serine	67	Citric acid	62	0,296	0,605	16,357	0,463	33	108	28	113	33	44 original
227	2	Serine	89	[775; Dopamine (4TMS)]	35	0,284	0,241	22,307	0,510	34	107	45	96	83	24 original
153	2	Serine	15	Alanine	62	0,283	0,111	15,221	0,456	35	106	57	84	22	47 original
268	2	Serine	130	Trehalose	61	0,281	0,456	20,869	0,389	36	105	36	105	72	83 original

142	2 Serine	4	Phosphoric acid	50	0.259	0.761	18.143	0.563	37	104	13	128	50	10 original
220	2 Serine	82	Lysine	39	0.255	0.590	11.064	0.596	38	103	30	111	7	4 original
217	2 Serine	79	Glucose	62	0.221	-0.020	26.260	0.441	39	102	65	76	110	58 original
202	2 Serine	64	[789; Tyramine (3TMS)]	61	0.220	0.092	18.186	0.341	40	101	60	81	53	127 original
199	2 Serine	61	[NA]	62	0.184	0.131	17.280	0.368	41	100	54	87	39	106 original
187	2 Serine	49	[877; Pyrophosphoric acid (4TMS)]	62	0.148	0.094	30.612	0.364	42	99	59	82	134	112 original
221	2 Serine	83	Sorbitol	56	0.145	0.617	9.668	0.569	43	98	26	115	3	9 original
246	2 Serine	108	Octadecanoic acid	62	0.144	0.395	18.861	0.359	44	97	39	102	55	116 original
269	2 Serine	51	[626; 5-Methylthioadenosine (3TMS)]	53	0.141	0.151	27.088	0.394	45	96	51	90	119	98 original
180	2 Serine	52	[NA]	44	0.114	0.153	25.840	0.418	46	95	50	91	105	78 original
233	2 Serine	95	[770; 3,4,6-Trisubstitutedphenylmethanolamine (5TMS)]	49	0.104	0.346	29.030	0.353	47	94	42	99	128	123 original
193	2 Serine	55	[612; 4-Aminobutyric acid (2TBS)]	43	0.103	0.139	34.346	0.597	48	93	52	89	140	3 original
209	2 Serine	71	[731; Erythrose (3TMS)]	62	0.102	0.469	13.060	0.463	49	92	35	106	9	45 original
276	2 Serine	138	[674; Ergosterol (1TMS)]	44	0.085	0.362	24.291	0.364	50	91	40	101	83	110 original
262	2 Serine	124	[734; 1-Monooleoylglycerol (2TMS); 1-Monoheptadecanoylglycerol (1TMS)]	57	0.079	0.532	33.353	0.390	51	90	34	107	139	104 original
261	2 Serine	123	[945; Galactofuranose-6-phosphate (7TMS)]	62	0.067	0.128	14.337	0.450	52	89	55	86	15	52 original
271	2 Serine	133	[655; Squalene]	62	0.038	0.425	15.904	0.388	53	88	37	104	25	95 original
249	2 Serine	111	[583; Erythritol (4TMS)]	41	0.029	0.094	27.771	0.259	54	87	58	83	121	137 original
256	2 Serine	118	[928; Glucopyranose-6-phosphate (6TMS)]	56	0.018	0.012	19.989	0.336	55	86	64	77	64	129 original
201	2 Serine	63	Glutamine	50	0.001	0.207	20.795	0.355	56	85	46	95	71	120 original
242	2 Serine	104	[795; Erythritol (4TMS)]	61	-0.004	0.017	18.139	0.437	57	84	63	78	49	82 original
251	2 Serine	113	Galactose-6-phosphate	60	-0.018	-0.162	21.760	0.406	58	83	72	69	79	84 original
277	2 Serine	139	[700; Ergosta-5,7-dien-3-ol]	38	-0.032	0.184	25.472	0.365	59	82	47	94	99	108 original
252	2 Serine	114	Fructose-6-phosphate	51	-0.037	-0.121	19.981	0.384	60	81	71	70	63	99 original
275	2 Serine	137	Ergosterol	62	-0.054	0.358	13.759	0.359	61	80	41	100	11	115 original
234	2 Serine	96	myo-Inositol	49	-0.058	-0.121	30.462	0.398	62	79	70	71	132	88 original
210	2 Serine	72	[919; D-Xylopyranose (4TMS)]	62	-0.080	-0.174	21.900	0.358	63	78	74	67	80	119 original
158	2 Serine	107	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.097	0.136	25.031	0.585	64	77	53	88	96	5 original
245	2 Serine	107	9-(Z)-Octadecanoic acid	62	-0.107	0.115	13.768	0.327	65	76	56	85	12	133 original
179	2 Serine	41	[639; Proline (2TMS)]	62	-0.111	-0.021	14.756	0.381	66	75	66	75	18	102 original
144	2 Serine	6	Glycerol	62	-0.112	-0.260	32.055	0.368	67	74	82	59	136	105 original
157	2 Serine	19	Alanine (BP) (3TMS)	62	-0.127	-0.117	16.232	0.364	68	73	69	72	28	111 original
257	2 Serine	119	[931; myo-Inositol-2-phosphate (7TMS)]	62	-0.131	0.019	17.463	0.365	69	71	62	79	41	109 original
173	2 Serine	35	Pyroglutamic acid	62	-0.131	-0.328	31.947	0.391	70	72	87	54	135	91 original
247	2 Serine	109	Octadecanoic acid	62	-0.155	0.157	18.172	0.338	71	70	49	92	52	128 original
218	2 Serine	80	[772; D-Glucose (5TMS)]	60	-0.164	-0.297	25.711	0.334	72	69	84	57	103	130 original
211	2 Serine	73	[708; Glucose methoxyamine (5TMS)]	56	-0.168	-0.200	22.665	0.467	73	68	75	66	84	42 original
191	2 Serine	53	Glycerol-2-phosphate	62	-0.172	-0.240	24.148	0.349	74	67	81	80	92	125 original
253	2 Serine	115	Glucose-6-phosphate	60	-0.173	-0.303	20.362	0.382	75	66	85	56	66	100 original
232	2 Serine	94	Hexadecanoic acid	62	-0.175	0.179	16.246	0.343	76	65	48	93	29	126 original
264	2 Serine	126	[559; Erythritol (4TMS)]	43	-0.181	-0.043	17.480	0.442	77	64	67	74	42	57 original
279	2 Serine	141	Lanosta-8,24-dien-3-beta-ol	59	-0.189	0.042	26.345	0.409	78	63	61	80	112	80 original
228	2 Serine	90	[910; 9-(Z)-Hexadecanoic acid (1TMS)]	62	-0.222	-0.203	17.606	0.331	79	61	76	65	43	131 original
214	2 Serine	76	Fructose	62	-0.222	-0.344	22.848	0.404	80	62	88	53	86	85 original
278	2 Serine	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	47	-0.230	-0.070	26.547	0.408	81	60	68	73	116	81 original
263	2 Serine	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	62	-0.234	-0.352	26.374	0.391	82	59	90	51	113	90 original
254	2 Serine	116	[882; Pseudouridine (5TMS)]	30	-0.237	-0.441	17.042	0.485	83	58	103	38	38	32 original
216	2 Serine	78	Mannose	60	-0.241	-0.368	24.874	0.358	84	57	92	49	95	117 original
156	2 Serine	18	[590; 1-Acetyl-2-thiohydantoin]	62	-0.243	-0.205	16.872	0.351	85	56	77	64	36	124 original

270	2 Serine	132 [895; Isomaltose methoxyamine (8TMS)]	40 -0.246	-0.513	25.728	0.245	86	55	108	33	104	139 original
229	2 Serine	91 [766; beta-D-Methylglucopyranoside (4TMS)]	62 -0.258	-0.720	28.090	0.473	87	54	137	4	129	38 original
208	2 Serine	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	55 -0.260	-0.211	14.420	0.410	88	53	78	63	16	79 original
185	2 Serine	47 [NA]	62 -0.267	-0.492	23.111	0.422	89	52	108	35	87	71 original
182	2 Serine	44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	48 -0.282	-0.229	18.778	0.355	90	51	80	61	54	121 original
265	2 Serine	127 [777; Fructose-6-phosphate methoxyamine (8TMS)]	37 -0.285	-0.395	15.414	0.149	91	50	96	45	23	140 original
166	2 Serine	28 Malic acid	62 -0.280	-0.535	16.769	0.444	92	49	110	31	35	56 original
259	2 Serine	121 [657; Erythritol (4TMS)]	53 -0.292	-0.228	25.509	0.381	93	48	79	62	101	101 original
240	2 Serine	102 [904; Galactose methoxyamine (5TMS)]	62 -0.298	-0.352	20.481	0.419	94	47	89	52	67	74 original
248	2 Serine	110 [715; Erythritol (4TMS)]	52 -0.302	-0.294	23.746	0.451	95	46	83	58	90	51 original
239	2 Serine	101 [832; Dopamine (4TMS)]	62 -0.302	-0.692	23.612	0.487	96	45	134	7	89	29 original
178	2 Serine	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	62 -0.305	-0.401	25.553	0.445	97	44	98	43	102	55 original
225	2 Serine	87 [945; beta-D-Glucopyranose (5TMS)]	60 -0.306	-0.391	28.294	0.380	98	43	95	46	124	103 original
223	2 Serine	85 [528; Methylenic acid (4TMS)]	48 -0.309	-0.491	16.354	0.576	99	42	105	36	32	6 original
258	2 Serine	120 [945; Uridine (3TMS)]	52 -0.309	-0.411	16.174	0.396	100	41	99	42	27	89 original
255	2 Serine	117 [724; Glycerol (3TMS)]	54 -0.315	-0.313	21.045	0.408	101	40	86	55	75	82 original
231	2 Serine	93 [607; Putrescine (4TMS)]	58 -0.318	-0.484	29.785	0.426	102	39	104	37	131	69 original
176	2 Serine	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	62 -0.319	-0.616	18.902	0.437	103	38	121	20	56	83 original
212	2 Serine	74 [912; Tetradecanoic acid (1TMS)]	62 -0.324	-0.168	22.288	0.415	104	37	73	68	82	77 original
244	2 Serine	108 [733; Threitol (4TMS)]	60 -0.324	-0.360	21.009	0.473	105	36	91	50	74	37 original
164	2 Serine	26 Citramalic acid	62 -0.325	-0.433	14.809	0.391	106	35	102	39	20	92 original
260	2 Serine	122 [644; Erythritol (4TMS)]	50 -0.334	-0.377	27.373	0.413	107	34	93	48	120	78 original
152	2 Serine	14 Fumaric acid	62 -0.337	-0.578	23.508	0.435	108	33	114	27	88	66 original
238	2 Serine	100 [857; Mannitol (6TMS)]	62 -0.340	-0.433	16.885	0.365	109	32	101	40	37	107 original
149	2 Serine	11 Succinic acid	62 -0.341	-0.559	17.878	0.418	110	31	112	29	47	75 original
241	2 Serine	103 [648; Ethylamine (2TMS)]	61 -0.368	-0.689	25.880	0.471	111	30	136	5	107	40 original
250	2 Serine	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (8TMS)]	61 -0.375	-0.426	29.016	0.401	112	29	100	41	127	86 original
273	2 Serine	135	62 -0.375	-0.384	14.529	0.355	113	28	94	47	17	122 original
159	2 Serine	21 [902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	62 -0.382	-0.552	16.560	0.447	114	27	111	30	34	53 original
154	2 Serine	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	62 -0.394	-0.688	18.954	0.481	115	26	132	9	57	35 original
224	2 Serine	86 [793; D-Galactono-1,4-lactone (4TMS)]	60 -0.395	-0.530	28.037	0.439	116	25	109	32	122	60 original
155	2 Serine	17 [700; 2-methyl-1,2-propanediol (2TMS)]	62 -0.398	-0.613	19.671	0.453	117	24	119	22	61	49 original
194	2 Serine	56 [828; Orotic acid (3TMS)]	62 -0.400	-0.608	26.707	0.435	118	23	117	24	118	64 original
162	2 Serine	24 [725; 2-Ketocyclohexanoic acid (2TMS)]	62 -0.401	-0.662	26.544	0.452	119	22	128	13	115	50 original
200	2 Serine	62 [812; D-Xylofuranose (4TMS)]	62 -0.402	-0.570	16.144	0.399	120	21	113	28	26	87 original
266	2 Serine	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	43 -0.406	-0.501	17.675	0.256	121	20	107	34	45	138 original
167	2 Serine	29 Erythritol	62 -0.407	-0.687	19.820	0.480	122	19	131	10	62	28 original
226	2 Serine	88 Gluconic acid	62 -0.408	-0.653	21.755	0.457	123	18	127	14	78	46 original
222	2 Serine	84 Mannitol	60 -0.409	-0.808	28.566	0.486	124	17	140	1	125	31 original
180	2 Serine	22 [690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	51 -0.429	-0.615	25.871	0.420	125	16	120	21	106	73 original
272	2 Serine	134 Isomaltose	62 -0.435	-0.623	26.283	0.430	126	15	122	19	111	67 original
184	2 Serine	46 Arabinose	62 -0.443	-0.595	25.953	0.428	127	14	116	25	108	68 original
177	2 Serine	39 [828; 1-Phenylethanol (1TMS)]	61 -0.454	-0.650	24.083	0.424	128	13	126	15	91	70 original
151	2 Serine	13 Uracil	50 -0.458	-0.681	20.736	0.481	129	12	130	11	70	36 original
235	2 Serine	97 [756; beta-D-Methylglucopyranoside (4TMS)]	62 -0.466	-0.690	26.394	0.435	130	11	133	8	114	65 original
150	2 Serine	12 Glycolic acid	61 -0.468	-0.834	25.330	0.407	131	10	124	17	97	83 original
230	2 Serine	92 [680; Glycerol-2-phosphate (4TMS)]	52 -0.468	-0.395	20.953	0.300	132	9	97	44	73	135 original
203	2 Serine	65 [646; 3-Deoxyglucitol (5TMS)]	61 -0.472	-0.608	28.597	0.421	133	8	118	23	126	72 original
182	2 Serine	54 [NA]	53 -0.488	-0.630	26.093	0.358	134	7	123	18	109	118 original

[illegible]

303	3 Ethanolamine	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	52	0.305	0.640	11,631	0.480	41	100	26	115	37	85 original
413	3 Ethanolamine	137	Ergosterol	62	0.243	0.388	17,637	0.373	42	99	48	93	80	138 original
339	3 Ethanolamine	63	Glutamine	50	0.241	0.712	10,488	0.606	43	98	19	122	21	18 original
395	3 Ethanolamine	119	[931; myo-Inositol-2-phosphate (7TMS)]	62	0.234	0.400	11,222	0.435	44	97	47	94	30	114 original
406	3 Ethanolamine	130	Trehalose	61	0.230	0.284	34,924	0.390	45	96	50	91	126	130 original
301	3 Ethanolamine	25	[709; 2,5-Diaminovalerolactam (2TMS)]	46	0.229	0.571	10,968	0.475	46	95	35	106	27	86 original
334	3 Ethanolamine	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	62	0.208	0.469	20,185	0.454	47	94	43	98	91	99 original
383	3 Ethanolamine	107	9-(Z)-Octadecenoic acid	62	0.200	0.405	19,136	0.410	48	93	45	96	87	125 original
319	3 Ethanolamine	43	[548; Leucine (2TBS)]	58	0.160	0.252	11,383	0.493	49	92	51	90	31	77 original
414	3 Ethanolamine	138	[674; Ergosterol (1TMS)]	44	0.154	0.209	10,393	0.416	50	91	54	87	19	121 original
417	3 Ethanolamine	141	Lanosta-8,24-dien-3-beta-ol	59	0.139	0.249	8,860	0.411	51	90	52	89	9	124 original
370	3 Ethanolamine	94	Hexadecanoic acid	62	0.129	0.099	26,286	0.482	52	89	58	83	111	82 original
387	3 Ethanolamine	111	[583; Erythritol (4TMS)]	40	0.126	0.030	12,030	0.388	53	88	62	79	42	132 original
385	3 Ethanolamine	109	Octadecanoic acid	62	0.113	-0.002	26,976	0.475	54	87	63	78	112	87 original
280	3 Ethanolamine	4	Phosphoric acid	50	0.107	0.361	35,846	0.385	55	86	49	92	127	134 original
415	3 Ethanolamine	139	[700; Ergosia-5,7-dien-3-ol]	36	0.060	0.186	12,175	0.341	56	85	55	88	44	140 original
359	3 Ethanolamine	83	Sorbitol	56	0.057	0.403	24,044	0.470	57	84	46	95	103	90 original
412	3 Ethanolamine	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	16	0.050	0.222	6,128	0.416	58	83	53	88	2	120 original
366	3 Ethanolamine	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	62	0.038	0.140	11,673	0.408	59	82	56	85	39	126 original
402	3 Ethanolamine	126	[559; Erythritol (4TMS)]	43	0.037	0.056	9,914	0.577	60	81	60	81	16	38 original
416	3 Ethanolamine	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	47	0.031	0.085	10,573	0.374	61	80	59	82	22	135 original
409	3 Ethanolamine	133	[855; Squalene]	62	0.013	0.132	11,565	0.346	62	79	57	84	34	138 original
340	3 Ethanolamine	64	[788; Tyramine (3TMS)]	61	-0.012	-0.231	9,489	0.432	63	78	68	73	14	115 original
348	3 Ethanolamine	72	[919; D-Xylopyranose (4TMS)]	62	-0.076	-0.079	10,899	0.343	64	77	64	77	26	139 original
372	3 Ethanolamine	96	myo-Inositol	48	-0.094	-0.126	14,013	0.369	65	76	66	75	58	137 original
369	3 Ethanolamine	93	[607; Putrescine (4TMS)]	58	-0.099	-0.288	13,006	0.436	66	75	72	69	50	112 original
329	3 Ethanolamine	53	Glycerol-2-phosphate	62	-0.104	-0.098	7,874	0.397	67	73	65	76	7	129 original
399	3 Ethanolamine	123	[945; Galactofuranose-6-phosphate (7TMS)]	82	-0.104	-0.385	16,539	0.595	68	74	80	61	76	27 original
411	3 Ethanolamine	135	[902; Melibiose (8TMS); alpha-D-Gal(1,6)-D-Glc (8TMS)]	62	-0.105	-0.204	17,385	0.415	69	72	67	74	78	122 original
392	3 Ethanolamine	116	[882; Pseudouridine (5TMS)]	29	-0.108	0.054	8,469	0.444	70	71	61	80	8	104 original
355	3 Ethanolamine	79	Glucose	62	-0.113	-0.579	40,722	0.620	71	70	97	44	135	11 original
291	3 Ethanolamine	15	Alanine	62	-0.117	-0.440	24,431	0.594	72	69	82	59	106	30 original
390	3 Ethanolamine	114	Fructose-6-phosphate	51	-0.125	-0.577	11,521	0.617	73	68	95	46	33	12 original
360	3 Ethanolamine	84	Mannitol	60	-0.130	-0.495	37,352	0.520	74	67	89	52	131	60 original
320	3 Ethanolamine	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	48	-0.147	-0.301	15,878	0.553	75	66	73	68	73	41 original
380	3 Ethanolamine	104	[795; Erythritol (4TMS)]	61	-0.158	-0.322	12,681	0.611	76	65	74	67	48	16 original
361	3 Ethanolamine	85	[528; Methylictric acid (4TMS)]	47	-0.177	-0.284	6,480	0.480	77	64	71	70	3	84 original
389	3 Ethanolamine	113	Galactose-6-phosphate	60	-0.180	-0.638	12,966	0.622	78	63	100	41	49	10 original
378	3 Ethanolamine	74	[912; Tetradecanoic acid (1TMS)]	62	-0.185	-0.278	13,765	0.449	79	62	70	71	56	101 original
350	3 Ethanolamine	102	[904; Galactose methoxyamine (5TMS)]	62	-0.186	-0.342	9,246	0.411	80	61	76	65	12	123 original
284	3 Ethanolamine	18	[590; 1-Acetyl-2-thiohydantoin]	62	-0.201	-0.335	13,185	0.404	81	60	75	66	53	128 original
394	3 Ethanolamine	118	[928; Glucopyranose-6-phosphate (8TMS)]	56	-0.205	-0.427	12,286	0.389	82	59	81	60	45	131 original
376	3 Ethanolamine	100	[857; Mannitol (6TMS)]	62	-0.217	-0.447	14,575	0.418	83	58	85	56	63	119 original
398	3 Ethanolamine	122	[644; Erythritol (4TMS)]	50	-0.220	-0.445	13,982	0.498	84	57	84	57	57	72 original
403	3 Ethanolamine	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	37	-0.222	-0.376	10,984	0.463	85	56	77	64	25	91 original
388	3 Ethanolamine	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	61	-0.223	-0.382	10,802	0.449	86	55	78	63	24	100 original
317	3 Ethanolamine	41	[639; Proline (2TMS)]	62	-0.231	-0.362	19,388	0.497	87	54	79	62	88	73 original
408	3 Ethanolamine	132	[895; Isomaltose methoxyamine (8TMS)]	40	-0.238	-0.594	14,973	0.423	88	53	99	42	85	118 original
386	3 Ethanolamine	110	[715; Erythritol (4TMS)]	52	-0.275	-0.523	15,316	0.607	89	52	90	51	69	17 original

393	3 Ethanolamine	117 [724; Glycerol (3TMS)]	54 -0.279	-0.463	13.577	0.511	90	51	86	55	55	68 original
396	3 Ethanolamine	120 [945; Uridine (3TMS)]	52 -0.299	-0.251	17.725	0.444	91	50	69	72	81	107 original
397	3 Ethanolamine	121 [657; Erythritol (4TMS)]	53 -0.299	-0.441	11.776	0.518	92	49	83	58	40	62 original
404	3 Ethanolamine	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	43 -0.309	-0.465	15.169	0.504	93	48	87	54	68	70 original
295	3 Ethanolamine	19 Alanine (BP) (3TMS)	62 -0.309	-0.552	18.297	0.561	94	47	92	49	83	38 original
391	3 Ethanolamine	115 Glucose-6-phosphate	60 -0.349	-0.724	30.944	0.554	95	46	108	33	118	40 original
311	3 Ethanolamine	35 Pyrogulamic acid	62 -0.353	-0.763	46.885	0.582	96	45	115	26	139	34 original
323	3 Ethanolamine	47 [NA]	62 -0.370	-0.466	16.214	0.439	97	44	88	53	75	108 original
316	3 Ethanolamine	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	62 -0.380	-0.568	39.608	0.528	98	43	93	48	134	58 original
349	3 Ethanolamine	73 [708; Glucose methoxamine (5TMS)]	56 -0.388	-0.572	14.190	0.534	99	42	94	47	61	55 original
302	3 Ethanolamine	26 Citramalic acid	62 -0.389	-0.578	21.757	0.445	100	41	96	45	95	103 original
297	3 Ethanolamine	21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	62 -0.396	-0.589	22.329	0.444	101	40	98	43	99	108 original
352	3 Ethanolamine	76 Fructose	62 -0.402	-0.773	32.347	0.587	102	39	118	23	120	33 original
288	3 Ethanolamine	12 Glycemic acid	61 -0.413	-0.655	9.959	0.424	103	38	103	38	17	117 original
382	3 Ethanolamine	108 [733; Threitol (4TMS)]	60 -0.417	-0.653	18.023	0.639	104	37	102	39	82	7 original
304	3 Ethanolamine	28 Malic acid	62 -0.419	-0.700	15.334	0.534	105	36	106	35	70	54 original
282	3 Ethanolamine	6 Glycerol	62 -0.425	-0.733	47.060	0.582	106	35	109	32	140	35 original
354	3 Ethanolamine	78 Mannose	60 -0.442	-0.690	15.455	0.516	107	34	105	36	71	64 original
298	3 Ethanolamine	22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	50 -0.450	-0.675	11.635	0.437	108	33	104	37	38	110 original
381	3 Ethanolamine	105 [705; 2-Ketogluconic acid (5TMS)]	46 -0.453	-0.642	19.132	0.551	109	32	101	40	86	42 original
401	3 Ethanolamine	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	62 -0.467	-0.816	38.303	0.593	110	31	125	16	133	31 original
367	3 Ethanolamine	91 [766; beta-D-Methylglucopyranoside (4TMS)]	62 -0.474	-0.722	24.364	0.544	111	30	107	34	105	46 original
346	3 Ethanolamine	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	56 -0.490	-0.549	23.879	0.532	112	29	91	50	102	57 original
280	3 Ethanolamine	14 Fumaric acid	62 -0.508	-0.734	9.758	0.483	113	28	110	31	15	80 original
287	3 Ethanolamine	11 Succinic acid	62 -0.512	-0.745	14.075	0.483	114	27	111	30	59	79 original
375	3 Ethanolamine	99 [662; Ribose-5-phosphate methoxamine (BP) (5TMS)]	39 -0.514	-0.746	12.083	0.514	115	26	112	29	43	66 original
368	3 Ethanolamine	92 [680; Glycerol-2-phosphate (4TMS)]	52 -0.517	-0.772	15.143	0.492	116	25	117	24	67	78 original
314	3 Ethanolamine	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	62 -0.520	-0.758	14.420	0.510	117	24	113	28	62	69 original
373	3 Ethanolamine	97 [756; beta-D-Methylglucopyranoside (4TMS)]	50 -0.523	-0.818	29.034	0.591	118	23	126	15	115	32 original
305	3 Ethanolamine	29 Erythritol	62 -0.528	-0.761	11.030	0.539	119	22	114	27	28	65 original
356	3 Ethanolamine	80 [772; D-Glucose (5TMS)]	60 -0.529	-0.783	37.219	0.539	120	21	120	21	128	52 original
9945	3 Ethanolamine	1 [938; Sulfuric acid (2TMS)]	34 -0.547	-0.813	12.364	0.588	121	20	123	18	46	25 duplicate
379	3 Ethanolamine	103 [648; Ethylamine (2TMS)]	61 -0.554	-0.768	22.205	0.564	122	19	116	25	98	37 original
338	3 Ethanolamine	62 [812; D-Xylofuranose (4TMS)]	62 -0.560	-0.803	20.233	0.540	123	18	122	19	92	51 original
377	3 Ethanolamine	101 [832; Dopamine (4TMS)]	62 -0.578	-0.777	18.400	0.548	124	17	119	22	84	43 original
315	3 Ethanolamine	39 [829; 1-Phenylethanol (1TMS)]	61 -0.580	-0.787	24.135	0.517	125	16	121	20	104	63 original
330	3 Ethanolamine	54 [NA]	53 -0.591	-0.814	14.082	0.499	126	15	124	17	60	71 original
382	3 Ethanolamine	86 [793; D-Galactono-1,4-lactone (4TMS)]	59 -0.612	-0.864	29.523	0.605	127	14	138	3	116	21 original
293	3 Ethanolamine	17 [700; 2-methyl-1,2-propanediol (2TMS)]	62 -0.613	-0.819	24.632	0.543	128	13	127	14	108	48 original
363	3 Ethanolamine	87 [945; beta-D-Glucopyranose (5TMS)]	60 -0.618	-0.830	41.347	0.545	129	12	131	10	136	45 original
333	3 Ethanolamine	57	53 -0.621	-0.830	21.849	0.534	130	11	132	9	96	56 original
364	3 Ethanolamine	88 Gluconic acid	62 -0.622	-0.828	19.779	0.596	131	9	130	11	90	26 original
332	3 Ethanolamine	56 [829; Oxalic acid (3TMS)]	62 -0.622	-0.866	17.553	0.611	132	10	139	2	79	15 original
300	3 Ethanolamine	24 [725; 2-Ketooctanoic acid (2TMS)]	62 -0.627	-0.847	38.222	0.614	133	8	133	8	132	13 original
292	3 Ethanolamine	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	62 -0.630	-0.827	24.469	0.595	134	7	129	12	107	28 original
410	3 Ethanolamine	134 Isomaltose	62 -0.634	-0.863	32.689	0.605	135	6	137	4	122	20 original
405	3 Ethanolamine	129 [840; Maltose methoxamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	57 -0.650	-0.858	19.092	0.595	136	5	136	5	85	29 original
322	3 Ethanolamine	46 Arabinose	62 -0.654	-0.877	25.890	0.602	137	4	140	1	110	23 original
341	3 Ethanolamine	65 [646; 3-Deoxyglucitol (5TMS)]	61 -0.660	-0.849	20.363	0.605	138	3	135	6	93	19 original



326	3 Ethanolamine	50	[746; Ribonic acid-1,4-lactone (3TMS)]	-0.822	14.685	0.495	139	2	128	13	64	76 original
289	3 Ethanolamine	62	Uracil	-0.848	23.650	0.613	140	1	134	7	101	14 original
488	4 Phosphoric acid	51	Lysine	0.685	5.096	0.558	1	140	5	138	1	4 original
449	4 Phosphoric acid	51	[596; N-Acetylglutamic acid (2TMS)]	0.778	6.465	0.560	2	139	1	140	3	2 original
471	4 Phosphoric acid	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	0.450	19.500	0.557	3	138	14	127	36	5 original
511	4 Phosphoric acid	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	0.430	39.140	0.442	4	137	16	125	125	26 original
10085	4 Phosphoric acid	2	Serine	0.761	18.143	0.563	5	136	2	139	31	1 duplicate
422	4 Phosphoric acid	51	Proline	0.704	11.579	0.559	6	135	4	137	14	3 original
440	4 Phosphoric acid	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	0.448	38.361	0.424	7	134	15	126	119	29 original
445	4 Phosphoric acid	32	[729; N,N-Dimethyllysine methyl ester]	0.571	35.373	0.448	8	133	8	133	108	24 original
479	4 Phosphoric acid	66	Glyceric acid-3-phosphate	0.619	32.775	0.480	9	132	7	134	90	11 original
552	4 Phosphoric acid	139	[700; Ergosta-5,7-dien-3-ol]	0.217	37.625	0.281	10	131	38	103	115	122 original
423	4 Phosphoric acid	51	Glycine	0.378	17.530	0.337	11	130	23	118	30	83 original
436	4 Phosphoric acid	51	Homoserine	0.359	28.833	0.449	12	128	27	114	68	23 original
428	4 Phosphoric acid	51	Alanine	0.108	19.301	0.357	13	129	46	95	34	65 original
481	4 Phosphoric acid	68	[570; Hypoxanthine (2TMS)]	0.395	26.798	0.349	14	127	20	121	57	76 original
444	4 Phosphoric acid	31	[622; Parabanic acid (2TMS)]	0.338	36.521	0.402	15	126	29	112	110	40 original
485	4 Phosphoric acid	72	[919; D-Xylopyranose (4TMS)]	0.115	34.829	0.354	16	125	44	97	103	70 original
531	4 Phosphoric acid	118	[928; Glucopyranose-6-phosphate (6TMS)]	0.134	32.329	0.311	17	124	40	101	89	104 original
492	4 Phosphoric acid	79	Glucose	0.033	9.203	0.459	18	123	58	83	11	19 original
543	4 Phosphoric acid	130	Trehalose	0.226	7.003	0.360	19	122	37	104	6	63 original
446	4 Phosphoric acid	33	Methionine	0.312	28.799	0.405	20	121	31	110	65	38 original
438	4 Phosphoric acid	25	[709; 2,5-Diaminovalerolactam (2TMS)]	0.362	30.408	0.437	21	120	25	116	78	27 original
521	4 Phosphoric acid	108	Octadecanoic acid	0.319	33.749	0.371	22	119	30	111	97	57 original
477	4 Phosphoric acid	64	[789; Tyramine (3TMS)]	0.063	32.156	0.279	23	118	55	88	88	124 original
443	4 Phosphoric acid	30	[815; Ethyl-3(2H)-thiophenone]	0.392	10.346	0.459	24	117	21	120	12	20 original
455	4 Phosphoric acid	42	Glutamic acid	0.551	11.901	0.500	25	116	9	132	16	9 original
472	4 Phosphoric acid	59	Ornithine; Arginine	0.450	6.629	0.473	26	115	13	128	5	12 original
494	4 Phosphoric acid	81	Tyrosine	0.480	7.176	0.455	27	114	11	130	7	21 original
10223	4 Phosphoric acid	3	Ethanolamine	0.361	35.846	0.385	28	113	26	115	107	48 duplicate
456	4 Phosphoric acid	43	[548; Leucine (2TBS)]	0.082	28.835	0.284	29	112	51	90	67	119 original
420	4 Phosphoric acid	7	Threonine	0.461	6.526	0.526	30	111	12	129	4	7 original
544	4 Phosphoric acid	131	[626; 5-Methylthioadenosine (3TMS)]	0.095	41.810	0.312	31	110	49	92	131	103 original
418	4 Phosphoric acid	5	Leucine	0.300	34.401	0.394	32	109	32	109	99	44 original
447	4 Phosphoric acid	34	Aspartic acid	0.274	7.693	0.374	33	108	34	107	9	53 original
493	4 Phosphoric acid	80	[772; D-Glucose (5TMS)]	-0.071	14.686	0.284	34	107	70	71	24	118 original
462	4 Phosphoric acid	49	[877; Pyrophosphoric acid (4TMS)]	0.130	45.991	0.324	35	106	42	99	136	98 original
458	4 Phosphoric acid	45	Homocysteine	0.126	47.274	0.334	36	105	43	98	138	89 original
421	4 Phosphoric acid	8	Isoleucine	0.659	17.359	0.548	37	104	6	135	29	6 original
490	4 Phosphoric acid	77	[826; beta-[(5-methyl-2-thienyl)methyleneamino]-benzeneacetic acid methyl ester]	0.518	10.639	0.465	38	103	10	131	13	16 original
517	4 Phosphoric acid	104	[795; Erythritol (4TMS)]	0.080	31.030	0.357	39	102	52	89	81	67 original
537	4 Phosphoric acid	124	[734; 1-Monooleoylglycerol (2TMS); 1-Monoheptadecanoylglycerol (1TMS)]	0.398	48.345	0.356	40	101	19	122	140	68 original
454	4 Phosphoric acid	41	[539; Proline (2TMS)]	0.023	22.597	0.276	41	100	59	82	45	126 original
536	4 Phosphoric acid	123	[945; Galactofuranose-6-phosphate (7TMS)]	0.110	24.985	0.421	42	99	45	96	54	30 original
482	4 Phosphoric acid	69	Arginine	0.339	16.659	0.418	43	98	28	113	28	32 original
450	4 Phosphoric acid	37	Phenylalanine	0.409	12.799	0.467	44	97	18	123	18	14 original
464	4 Phosphoric acid	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	0.413	43.674	0.387	45	96	17	124	132	47 original
432	4 Phosphoric acid	19	Alanine (BP) (3TMS)	-0.022	25.365	0.334	46	95	63	78	55	90 original

419	4	Phosphoric acid	6	Glycerol	51	0.015	-0.081	7.421	0.256	47	94	72	69	8	134	original
461	4	Phosphoric acid	48	Asparagine	51	0.010	-0.167	30.393	0.326	48	83	39	102	77	97	original
485	4	Phosphoric acid	82	Lysine	38	0.007	0.105	21.539	0.351	49	92	47	94	41	74	original
486	4	Phosphoric acid	83	Sorbitol	51	-0.001	0.734	13.987	0.504	50	91	3	138	22	8	original
468	4	Phosphoric acid	55	[612; 4-Aminobutyric acid (2TBS)]	41	-0.005	-0.065	47.705	0.418	51	90	68	73	139	33	original
551	4	Phosphoric acid	138	[674; Ergosterol (1TMS)]	35	-0.008	0.133	36.563	0.393	52	89	41	100	112	45	original
473	4	Phosphoric acid	60	Glycerol-3-phosphate	51	-0.009	0.387	13.944	0.466	53	88	22	119	21	15	original
460	4	Phosphoric acid	47	[NA]	51	-0.020	-0.263	34.100	0.365	54	87	95	46	98	59	original
524	4	Phosphoric acid	111	[583; Erythritol (4TMS)]	33	-0.030	-0.024	40.682	0.264	55	86	64	77	128	131	original
546	4	Phosphoric acid	133	[855; Squalene]	51	-0.031	0.277	29.710	0.389	56	85	33	108	71	46	original
480	4	Phosphoric acid	67	Citric acid	51	-0.032	0.382	12.155	0.413	57	84	24	117	17	34	original
527	4	Phosphoric acid	114	Fructose-6-phosphate	40	-0.033	-0.035	32.089	0.300	58	83	65	76	87	111	original
474	4	Phosphoric acid	61	[NA]	51	-0.034	-0.072	31.263	0.261	59	82	71	70	82	133	original
550	4	Phosphoric acid	137	Ergosterol	51	-0.040	0.236	23.426	0.405	60	81	36	105	48	36	original
553	4	Phosphoric acid	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	41	-0.041	0.000	40.588	0.381	61	80	61	80	127	50	original
538	4	Phosphoric acid	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	51	-0.048	-0.157	13.910	0.274	62	79	80	61	20	127	original
483	4	Phosphoric acid	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	48	-0.057	-0.163	18.237	0.350	63	78	82	59	32	75	original
500	4	Phosphoric acid	87	[945; beta-D-Glucopyranose (5TMS)]	51	-0.062	-0.186	13.806	0.278	64	77	84	57	19	125	original
20																
433	4	Phosphoric acid	107	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	30	-0.062	-0.086	36.549	0.364	65	76	73	68	111	60	original
520	4	Phosphoric acid	109	9-(Z)-Octadecenoic acid	51	-0.073	0.091	21.518	0.329	66	75	50	91	40	95	original
554	4	Phosphoric acid	141	Lanosta-8,24-dien-3-beta-ol	50	-0.082	0.016	40.925	0.371	67	74	60	81	129	56	original
530	4	Phosphoric acid	117	[724; Glycerol (3TMS)]	43	-0.083	-0.135	31.489	0.348	68	73	77	64	85	77	original
466	4	Phosphoric acid	53	Glycerol-2-phosphate	51	-0.084	-0.191	39.137	0.282	69	72	85	56	124	121	original
491	4	Phosphoric acid	78	Mannose	50	-0.086	-0.150	36.975	0.353	70	71	79	62	113	71	original
509	4	Phosphoric acid	96	myo-Inositol	42	-0.094	-0.197	44.634	0.269	71	70	87	54	135	128	original
431	4	Phosphoric acid	18	[590; 1-Acetyl-2-thiohydantoin]	51	-0.095	-0.050	28.933	0.302	72	69	67	74	68	108	original
534	4	Phosphoric acid	121	[657; Erythritol (4TMS)]	43	-0.096	-0.112	38.621	0.283	73	68	75	66	122	120	original
502	4	Phosphoric acid	89	[776; Dopamine (4TMS)]	31	-0.110	0.099	33.429	0.372	74	67	48	93	95	54	original
503	4	Phosphoric acid	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	51	-0.111	-0.137	30.289	0.333	75	66	78	63	76	91	original
448	4	Phosphoric acid	35	Pyroglutamic acid	51	-0.112	-0.175	7.749	0.297	76	65	83	58	10	112	original
533	4	Phosphoric acid	120	[945; Uridine (3TMS)]	41	-0.112	-0.214	21.581	0.316	77	64	92	49	42	101	original
526	4	Phosphoric acid	113	Galactose-6-phosphate	49	-0.112	-0.111	35.089	0.371	78	63	74	67	105	55	original
529	4	Phosphoric acid	116	[892; Pseudouridine (5TMS)]	30	-0.117	-0.430	28.792	0.358	79	62	122	19	64	64	original
532	4	Phosphoric acid	119	[931; myo-Inositol-2-phosphate (7TMS)]	51	-0.123	-0.041	30.174	0.310	80	61	66	75	73	105	original
508	4	Phosphoric acid	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	38	-0.127	0.075	41.400	0.353	81	60	53	88	130	72	original
489	4	Phosphoric acid	76	Fructose	51	-0.128	-0.200	18.265	0.339	82	59	88	53	33	82	original
507	4	Phosphoric acid	94	Hexadecanoic acid	51	-0.131	0.072	16.503	0.294	83	58	54	87	27	113	original
465	4	Phosphoric acid	52	[NA]	33	-0.133	-0.015	37.756	0.451	84	57	62	79	117	22	original
519	4	Phosphoric acid	108	[733; Threitol (4TMS)]	49	-0.136	-0.207	30.657	0.413	85	56	90	51	79	35	original
522	4	Phosphoric acid	109	Octadecanoic acid	51	-0.137	0.056	19.334	0.315	86	55	57	84	35	102	original
486	4	Phosphoric acid	73	[708; Glucose methoxamine (5TMS)]	50	-0.138	-0.276	36.061	0.342	87	54	96	45	109	79	original
484	4	Phosphoric acid	71	[731; Erythrose (3TMS)]	51	-0.144	0.238	23.032	0.462	88	53	35	106	47	17	original
439	4	Phosphoric acid	26	Citramalic acid	51	-0.150	-0.276	19.792	0.356	89	51	97	44	37	69	original
504	4	Phosphoric acid	81	[766; beta-D-Methylglucopyranoside (4TMS)]	51	-0.150	-0.549	35.972	0.471	90	52	136	5	108	13	original
427	4	Phosphoric acid	14	Fumaric acid	51	-0.151	-0.374	37.743	0.379	91	49	108	33	116	52	original
514	4	Phosphoric acid	101	[832; Dopamine (4TMS)]	51	-0.151	-0.467	33.392	0.447	92	50	125	16	94	25	original
434	4	Phosphoric acid	121	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	51	-0.153	-0.309	20.608	0.360	93	48	103	38	38	62	original
535	4	Phosphoric acid	122	[844; Erythritol (4TMS)]	39	-0.155	-0.244	38.295	0.380	94	47	93	48	118	51	original
498	4	Phosphoric acid	85	[529; Methylcitric acid (4TMS)]	47	-0.156	-0.209	31.353	0.405	95	46	91	50	84	37	original
475	4	Phosphoric acid	62	[812; D-Xylofuranose (4TMS)]	51	-0.159	-0.343	22.855	0.291	96	45	107	34	46	114	original

499	4 Phosphoric acid	86	[793; D-Galactono-1,4-lactone (4TMS)]	49	-0.163	-0.293	30.235	0.352	97	44	100	41	74	73 original
476	4 Phosphoric acid	63	Glutamine	39	-0.163	0.059	32.996	0.200	98	43	56	85	91	138 original
453	4 Phosphoric acid	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	51	-0.169	-0.252	5.541	0.396	99	42	94	47	2	43 original
441	4 Phosphoric acid	28	Malic acid	51	-0.170	-0.343	27.450	0.401	100	41	106	35	59	41 original
426	4 Phosphoric acid	13	Uracil	51	-0.172	-0.480	24.734	0.337	101	40	127	14	52	84 original
523	4 Phosphoric acid	110	[715; Erythritol (4TMS)]	41	-0.173	-0.161	33.707	0.432	102	39	81	60	96	28 original
539	4 Phosphoric acid	128	[559; Erythritol (4TMS)]	33	-0.178	-0.066	27.586	0.420	103	38	69	72	60	31 original
528	4 Phosphoric acid	115	Glucose-6-phosphate	49	-0.179	-0.195	14.632	0.288	104	37	86	55	23	117 original
487	4 Phosphoric acid	74	[912; Tetradecanoic acid (1TMS)]	51	-0.186	-0.122	34.460	0.363	105	36	76	65	100	61 original
469	4 Phosphoric acid	56	[829; Citric acid (3TMS)]	51	-0.198	-0.310	36.389	0.301	106	35	114	27	120	110 original
424	4 Phosphoric acid	11	Succinic acid	51	-0.202	-0.380	29.548	0.323	107	34	109	32	69	99 original
549	4 Phosphoric acid	138	[748; D-Sedoheptulose-7-phosphate (7TMS)]	13	-0.205	-0.434	15.246	0.335	108	33	123	18	26	88 original
430	4 Phosphoric acid	17	[700; 2-methyl-1,2-propanediol (2TMS)]	51	-0.206	-0.428	22.517	0.318	109	32	121	20	44	100 original
478	4 Phosphoric acid	65	[646; 3-Deoxyglucitol (5TMS)]	50	-0.207	-0.397	36.931	0.281	110	30	113	28	123	123 original
452	4 Phosphoric acid	39	[828; 1-Phenylethanol (1TMS)]	50	-0.207	-0.427	26.658	0.331	111	31	119	22	63	92 original
516	4 Phosphoric acid	103	[648; Ethylamine (2TMS)]	50	-0.213	-0.476	33.003	0.403	112	29	126	15	92	39 original
463	4 Phosphoric acid	50	[746; Ribonic acid-1,4-lactone (3TMS)]	48	-0.216	-0.494	46.393	0.329	113	28	130	11	137	94 original
		129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	46	-0.223	-0.417	34.463	0.265	114	27	116	25	101	130 original
542	4 Phosphoric acid	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	51	-0.224	-0.428	30.267	0.302	115	26	120	21	75	109 original
451	4 Phosphoric acid	46	Arabinose	51	-0.227	-0.392	30.734	0.290	116	24	112	29	80	115 original
547	4 Phosphoric acid	134	Isomaltose	51	-0.227	-0.416	22.198	0.330	117	25	115	26	43	93 original
429	4 Phosphoric acid	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	51	-0.230	-0.498	21.365	0.337	118	23	132	9	39	85 original
501	4 Phosphoric acid	88	Gluconic acid	51	-0.231	-0.493	26.662	0.369	119	22	129	12	70	58 original
437	4 Phosphoric acid	24	[725; 2-Ketocitric acid (2TMS)]	51	-0.236	-0.459	11.598	0.328	120	21	124	17	15	96 original
457	4 Phosphoric acid	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	38	-0.249	-0.206	27.051	0.357	121	20	89	52	58	66 original
545	4 Phosphoric acid	132	[895; Isomaltose methoxyamine (8TMS)]	30	-0.251	-0.364	34.933	0.217	122	19	111	30	104	136 original
435	4 Phosphoric acid	22	[690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	39	-0.255	-0.424	37.388	0.340	123	18	118	23	114	81 original
515	4 Phosphoric acid	102	[904; Galactose methoxyamine (5TMS)]	51	-0.256	-0.301	34.535	0.310	124	17	102	39	102	106 original
442	4 Phosphoric acid	28	Erythritol	51	-0.266	-0.526	33.041	0.346	125	16	135	6	93	78 original
525	4 Phosphoric acid	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	50	-0.282	-0.294	44.289	0.337	126	15	101	40	134	88 original
497	4 Phosphoric acid	84	Mannitol	49	-0.294	-0.761	14.826	0.460	127	14	140	1	25	18 original
513	4 Phosphoric acid	100	[857; Mannitol (6TMS)]	51	-0.296	-0.310	28.073	0.305	128	13	104	37	62	107 original
9946	4 Phosphoric acid	1	[938; Sulfuric acid (2TMS)]	24	-0.297	-0.630	25.742	0.261	129	12	139	2	56	132-tuplicate
425	4 Phosphoric acid	12	Glyceric acid	50	-0.309	-0.481	39.653	0.335	130	11	128	13	128	87 original
470	4 Phosphoric acid	57	[757; 2-Desoxy-pentos-3-ylose dimethoxyamine (2TMS)]	42	-0.310	-0.381	30.127	0.273	131	10	110	31	72	128 original
		135												
548	4 Phosphoric acid	54	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (6TMS)]	51	-0.315	-0.292	23.664	0.341	132	9	99	42	50	80 original
467	4 Phosphoric acid	43	[NA]	43	-0.340	-0.503	36.610	0.290	133	8	133	8	121	116 original
540	4 Phosphoric acid	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	27	-0.362	-0.342	23.496	0.136	134	7	105	36	49	140 original
505	4 Phosphoric acid	92	[680; Glycerol-2-phosphate (4TMS)]	42	-0.366	-0.278	31.883	0.236	135	6	98	43	86	135 original
510	4 Phosphoric acid	97	[756; beta-D-Methylglucopyranoside (4TMS)]	40	-0.374	-0.497	24.694	0.396	136	5	131	10	51	42 original
506	4 Phosphoric acid	93	[607; Putrescine (4TMS)]	48	-0.385	-0.597	44.195	0.482	137	4	138	3	133	10 original
541	4 Phosphoric acid	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	33	-0.413	-0.419	24.854	0.205	138	3	117	24	53	137 original
512	4 Phosphoric acid	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	29	-0.429	-0.515	31.306	0.191	139	2	134	7	83	139 original
518	4 Phosphoric acid	105	[705; 2-Ketogluconic acid (5TMS)]	36	-0.486	-0.584	27.851	0.382	140	1	137	4	61	49 original
559	5 Leucine	10	Glycine	45	0.772	0.858	19.255	0.556	1	140	9	132	103	34 original
579	5 Leucine	30	[816; Ethyl-3(2H)-thiophenone]	45	0.762	0.866	29.727	0.601	2	139	5	136	127	13 original
638	5 Leucine	89	[775; Dopamine (4TMS)]	29	0.749	0.740	9.829	0.520	3	138	21	120	18	61 original
591	5 Leucine	42	Glutamic acid	44	0.702	0.855	29.872	0.652	4	137	10	131	128	4 original

600	5 Leucine	51	[498; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	38	0.684	0.818	12,795	0.585	5	136	14	127	49	21 original
630	5 Leucine	81	Tyrosine	45	0.879	0.694	34,238	0.597	6	135	24	117	135	15 original
582	5 Leucine	33	Methionine	45	0.673	0.840	9,719	0.641	7	134	11	130	17	6 original
597	5 Leucine	48	Asparagine	45	0.653	0.880	10,162	0.487	8	133	25	116	21	79 original
631	5 Leucine	82	Lysine	38	0.847	0.866	15,396	0.550	9	132	6	135	73	37 original
644	5 Leucine	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	35	0.844	0.652	13,158	0.599	10	131	27	114	55	14 original
618	5 Leucine	69	Arginine	45	0.636	0.891	21,453	0.637	11	130	2	139	109	8 original
617	5 Leucine	68	[570; Hypoxanthine (2TMS)]	16	0.633	0.859	9,078	0.557	12	129	8	133	12	33 original
10224	5 Leucine	61	[NA]	45	0.628	0.457	8,704	0.348	13	128	37	104	11	118 original
557	5 Leucine	3	Ethanolamine	44	0.619	0.598	6,613	0.525	14	127	30	111	3	53 duplicate
604	5 Leucine	8	Isoleucine	45	0.616	0.861	19,616	0.545	15	126	7	134	104	40 original
		55	[612; 4-Aminobutyric acid (2TBS)]	39	0.609	0.593	17,014	0.474	16	125	32	109	88	86 original
		77	[826; beta-[(5-methyl-2-thienyl)methyl]eneamino-benzeneacetic acid methyl ester]	45	0.608	0.777	30,367	0.592	17	124	18	123	130	17 original
626	5 Leucine	45	Homocysteine	43	0.608	0.744	13,613	0.543	18	123	20	121	60	43 original
594	5 Leucine	49	[877; Pyrophosphoric acid (4TMS)]	45	0.604	0.745	10,713	0.496	19	122	19	122	28	75 original
598	5 Leucine	52	[NA]	28	0.593	0.543	11,801	0.574	20	121	33	108	36	26 original
601	5 Leucine	34	Aspartic acid	45	0.580	0.810	31,761	0.628	21	120	16	125	131	12 original
583	5 Leucine	9	Proline	45	0.574	0.874	28,751	0.637	22	119	4	137	122	9 original
558	5 Leucine	25	[709; 2,5-Diaminovalerolactam (2TMS)]	29	0.562	0.837	7,304	0.571	23	118	12	129	5	29 original
574	5 Leucine	131	[826; 5-Methylthioadenosine (3TMS)]	40	0.546	0.656	10,082	0.495	24	117	26	115	19	77 original
680	5 Leucine	59	Ornithine; Arginine	45	0.537	0.819	38,973	0.595	25	116	13	128	140	16 original
608	5 Leucine	32	[728; N,N-Dimethyllysine methyl ester]	45	0.523	0.906	4,860	0.721	26	115	1	140	1	2 original
581	5 Leucine	37	Phenylalanine	45	0.467	0.600	23,112	0.505	27	114	29	112	112	69 original
586	5 Leucine	31	[622; Parabanic acid (2TMS)]	45	0.465	0.630	8,949	0.567	28	113	28	113	4	30 original
580	5 Leucine	20												
569	5 Leucine		[619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	29	0.453	0.722	10,569	0.573	29	112	22	119	27	27 original
572	5 Leucine	23	Homoserine	45	0.442	0.815	9,340	0.677	30	111	15	126	15	3 original
612	5 Leucine	63	Glutamine	34	0.405	0.530	11,806	0.412	31	110	34	107	37	103 original
10086	5 Leucine	2	Serine	45	0.396	0.803	19,635	0.640	32	109	17	124	105	7 duplicate
633	5 Leucine	84	Mannitol	43	0.367	0.389	21,648	0.507	33	108	38	103	110	68 original
616	5 Leucine	67	Citric acid	45	0.341	0.249	23,948	0.458	34	107	42	99	115	81 original
657	5 Leucine	108	Octadecanoic acid	45	0.339	0.377	8,170	0.392	35	106	39	102	7	110 original
642	5 Leucine	93	[607; Putrescine (4TMS)]	42	0.310	0.108	12,943	0.483	36	105	50	91	51	82 original
615	5 Leucine	66	Glyceric acid-3-phosphate	45	0.285	0.488	8,396	0.574	37	104	36	105	10	25 original
592	5 Leucine	43	[548; Leucine (2TBS)]	44	0.281	0.597	8,236	0.451	38	103	31	110	8	93 original
609	5 Leucine	60	Glycerol-3-phosphate	45	0.275	0.181	22,707	0.484	39	102	47	94	111	80 original
556	5 Leucine	7	Threonine	45	0.269	0.510	28,560	0.630	40	101	35	106	128	11 original
576	5 Leucine	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	43	0.231	0.875	6,328	0.646	41	100	3	138	2	5 original
639	5 Leucine	90	[910; 9-(Z)-Hexadecanoic acid (1TMS)]	45	0.194	0.096	10,257	0.341	42	99	51	90	22	123 original
656	5 Leucine	107	9-(Z)-Octadecanoic acid	45	0.172	0.163	15,989	0.347	43	98	48	93	77	120 original
647	5 Leucine	98	[897; Ribose-5-phosphate methoxyamine (5TMS)]	33	0.159	0.720	10,121	0.728	44	97	23	118	20	1 original
602	5 Leucine	53	Glycerol-2-phosphate	45	0.123	0.208	9,181	0.332	45	96	43	98	13	125 original
668	5 Leucine	119	[931; myo-inositol-2-phosphate (7TMS)]	45	0.099	-0.038	11,668	0.368	46	95	55	86	33	115 original
10361	5 Leucine	4	Phosphoric acid	44	0.089	0.300	34,401	0.394	47	94	41	100	136	108 duplicate
624	5 Leucine	75	Lysine	45	0.081	0.338	38,215	0.551	48	93	40	101	139	36 original
621	5 Leucine	72	[919; D-Xylopyranose (4TMS)]	45	0.034	0.193	9,568	0.394	49	92	45	96	16	109 original
596	5 Leucine	47	[NA]	45	0.022	0.191	10,290	0.428	50	91	46	95	24	99 original
585	5 Leucine	36	[596; N-Acetylglutamic acid (2TMS)]	45	0.012	0.207	29,311	0.581	51	90	44	97	125	32 original
679	5 Leucine	130	Trehalose	44	-0.040	0.067	28,046	0.385	52	89	52	89	124	112 original

673	5 Leucine	124	[734; 1-Monooxyglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	41	-0.051	-0.103	15.734	0.413	53	88	57	84	75	102	original
685	5 Leucine	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	11	-0.055	-0.038	8.245	0.019	54	87	54	87	9	140	original
9947	5 Leucine	1	[938; Sulfuric acid (2TMS)]	18	-0.059	-0.297	8.154	0.162	55	86	64	77	6	136	duplicate
688	5 Leucine	139	[700; Ergosta-5,7-dien-3-ol]	27	-0.071	0.034	11.678	0.128	56	85	53	88	34	138	original
660	5 Leucine	111	[583; Erythritol (4TMS)]	27	-0.083	-0.147	11.935	0.232	57	84	60	81	40	132	original
686	5 Leucine	137	Ergosterol	45	-0.091	-0.322	16.981	0.447	58	83	65	76	87	96	original
620	5 Leucine	71	[731; Erythrose (3TMS)]	45	-0.115	-0.393	14.933	0.523	59	82	69	72	70	57	original
564	5 Leucine	15	Alanine	45	-0.117	-0.120	19.903	0.544	60	81	59	82	106	42	original
607	5 Leucine	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	45	-0.133	0.120	18.538	0.572	61	80	49	92	100	28	original
613	5 Leucine	64	[789; Tyramine (3TMS)]	44	-0.142	-0.053	9.311	0.273	62	79	56	85	14	130	original
690	5 Leucine	141	Lanosta-8,24-dien-3-beta-ol	45	-0.145	-0.373	12.525	0.400	63	78	67	74	46	105	original
645	5 Leucine	96	myo-Inositol	39	-0.155	-0.116	14.813	0.194	64	77	58	83	68	134	original
684	5 Leucine	135		45	-0.184	-0.518	14.445	0.484	65	76	78	63	66	81	original
689	5 Leucine	140	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	38	-0.188	-0.331	12.627	0.379	66	75	68	75	47	114	original
665	5 Leucine	116	[882; Pseudouridine (5TMS)]	27	-0.219	-0.378	12.335	0.172	67	74	68	73	43	135	original
640	5 Leucine	91	[766; beta-D-Methylglucopyranoside (4TMS)]	45	-0.238	-0.196	11.845	0.521	68	73	61	80	39	60	original
628	5 Leucine	79	Glucose	45	-0.238	-0.397	33.347	0.477	69	72	70	71	134	84	original
681	5 Leucine	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (8TMS)]	44	-0.245	-0.530	12.951	0.519	70	71	79	62	52	63	original
658	5 Leucine	109	Octadecanoic acid	45	-0.259	-0.787	26.966	0.517	71	70	119	22	120	64	original
643	5 Leucine	94	Hexadecanoic acid	45	-0.273	-0.708	24.748	0.470	72	69	98	43	117	89	original
651	5 Leucine	102	[904; Galactose methoxamine (5TMS)]	45	-0.281	-0.538	10.276	0.463	73	68	80	61	23	90	original
687	5 Leucine	138	[674; Ergosterol (1TMS)]	32	-0.294	-0.448	11.629	0.356	74	67	72	69	32	117	original
634	5 Leucine	85	[529; Methylnic acid (4TMS)]	45	-0.313	-0.618	10.380	0.471	75	66	91	50	25	88	original
649	5 Leucine	100	[857; Mammilol (6TMS)]	45	-0.321	-0.665	12.852	0.474	76	65	96	45	50	87	original
667	5 Leucine	118	[928; Glucopyranose-6-phosphate (6TMS)]	39	-0.323	-0.245	11.836	0.273	77	64	62	79	38	129	original
561	5 Leucine	12	Glyceric acid	44	-0.340	-0.772	11.961	0.532	78	63	112	29	41	49	original
669	5 Leucine	120	[945; Uridine (3TMS)]	35	-0.358	-0.248	14.196	0.545	79	62	63	78	64	39	original
650	5 Leucine	101	[832; Dopamine (4TMS)]	45	-0.360	-0.422	11.508	0.512	80	61	71	70	31	68	original
646	5 Leucine	97	[756; beta-D-Methylglucopyranoside (4TMS)]	33	-0.383	-0.472	16.463	0.348	81	60	73	68	83	119	original
623	5 Leucine	74	[912; Tetradecanoic acid (1TMS)]	45	-0.390	-0.757	16.423	0.589	82	59	108	33	82	18	original
682	5 Leucine	133	[855; Squalene]	45	-0.418	-0.504	12.474	0.445	83	58	76	65	44	97	original
652	5 Leucine	103	[648; Ethylamine (2TMS)]	44	-0.467	-0.617	14.535	0.525	84	57	90	51	67	52	original
677	5 Leucine	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	26	-0.471	-0.588	13.184	0.152	85	56	85	56	58	137	original
632	5 Leucine	83	Sorbitol	45	-0.493	-0.718	23.492	0.535	86	55	100	41	113	47	original
587	5 Leucine	18	[590; 1-Acetyl-2-thiohydantoin]	45	-0.495	-0.649	12.498	0.488	87	54	92	49	45	78	original
654	5 Leucine	105	[705; 2-Ketogluconic acid (5TMS)]	29	-0.498	-0.718	13.083	0.424	88	53	101	40	54	101	original
555	5 Leucine	6	Glycerol	45	-0.501	-0.605	37.909	0.335	89	52	87	54	138	124	original
641	5 Leucine	92	[690; Glycerol-2-phosphate (4TMS)]	35	-0.503	-0.477	13.489	0.227	90	51	74	67	58	133	original
578	5 Leucine	29	Erythritol	45	-0.509	-0.844	10.511	0.588	91	49	126	15	26	20	original
587	5 Leucine	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	45	-0.509	-0.852	12.652	0.524	92	50	129	12	48	55	original
560	5 Leucine	11	Succinic acid	45	-0.511	-0.734	12.021	0.496	93	48	103	38	42	76	original
676	5 Leucine	127	[777; Fructose-6-phosphate methoxamine (6TMS)]	21	-0.524	-0.580	11.259	0.075	94	47	84	57	29	139	original
681	5 Leucine	132	[895; Isomaltose methoxamine (8TMS)]	25	-0.527	-0.758	17.231	0.258	95	46	110	31	89	131	original
593	5 Leucine	44	[910; 2-Ketogluconic acid methoxamine (4TMS)]	31	-0.527	-0.798	16.857	0.427	96	45	118	23	86	100	original
629	5 Leucine	80	[772; D-Glucose (5TMS)]	43	-0.530	-0.492	27.924	0.342	97	44	75	68	121	122	original
675	5 Leucine	126	[559; Erythritol (4TMS)]	28	-0.538	-0.792	13.693	0.474	98	43	116	25	61	85	original
662	5 Leucine	113	Galactose-6-phosphate	43	-0.539	-0.598	13.912	0.411	99	41	86	55	62	104	original
664	5 Leucine	115	Galactose-6-phosphate	43	-0.539	-0.679	24.922	0.397	100	42	97	44	118	107	original

674	5 Leucine	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	45	-0.543	-0.565	29,990	0.388	101	39	82	59	129	111	original
570	5 Leucine	21	[878; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	45	-0.543	-0.755	17,856	0.543	102	40	105	36	95	44	original
577	5 Leucine	28	Malic acid	45	-0.545	-0.851	13,196	0.583	103	38	128	13	57	22	original
672	5 Leucine	123	[845; Galactofuranose-6-phosphate (7TMS)]	45	-0.552	-0.517	14,829	0.478	104	37	77	64	69	83	original
584	5 Leucine	35	Pyroglutamic acid	45	-0.554	-0.655	37,562	0.448	105	36	93	48	137	95	original
663	5 Leucine	114	Fructose-6-phosphate	34	-0.554	-0.615	12,980	0.345	106	35	89	52	53	121	original
603	5 Leucine	54	[NA]	36	-0.556	-0.860	14,223	0.285	107	33	94	47	65	127	original
565	5 Leucine	16	[844; 2-Methyl-1,3-butanediol (2TMS)]	45	-0.556	-0.662	18,333	0.556	108	34	133	8	98	35	original
566	5 Leucine	17	[700; 2-methyl-1,2-propanediol (2TMS)]	45	-0.568	-0.755	18,366	0.449	109	32	106	35	99	94	original
648	5 Leucine	99	[662; Ribose-5-phosphate methoxamine (BP) (5TMS)]	22	-0.576	-0.822	11,780	0.323	110	31	124	17	35	128	original
636	5 Leucine	87	[945; beta-D-Glucopyranose (5TMS)]	45	-0.578	-0.549	32,599	0.274	111	30	81	60	133	128	original
573	5 Leucine	24	[725; 2-Ketooctanoic acid (2TMS)]	45	-0.582	-0.861	28,827	0.540	112	29	132	9	123	46	original
589	5 Leucine	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	45	-0.584	-0.864	32,108	0.633	113	28	134	7	132	10	original
619	5 Leucine	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	44	-0.586	-0.566	20,175	0.359	114	27	83	58	108	116	original
653	5 Leucine	104	[795; Erythritol (4TMS)]	45	-0.590	-0.766	14,137	0.525	115	26	111	30	63	51	original
563	5 Leucine	14	Fumaric acid	45	-0.592	-0.846	11,382	0.589	116	25	127	14	30	19	original
575	5 Leucine	26	Citramalic acid	45	-0.598	-0.778	17,597	0.512	117	24	113	28	92	67	original
605	5 Leucine	56	[829; Oxalic acid (3TMS)]	45	-0.602	-0.792	16,364	0.499	118	23	117	24	80	74	original
588	5 Leucine	39	[829; 1-Phenylethanol (1TMS)]	44	-0.607	-0.860	18,699	0.524	119	22	131	10	101	56	original
637	5 Leucine	88	Gluconic acid	45	-0.616	-0.806	14,996	0.534	120	21	120	21	71	48	original
571	5 Leucine	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	36	-0.622	-0.858	13,598	0.545	121	20	130	11	59	41	original
625	5 Leucine	76	Fructose	45	-0.626	-0.729	26,053	0.542	122	19	102	39	119	45	original
614	5 Leucine	65	[846; 3-Deoxyglucitol (5TMS)]	44	-0.628	-0.818	18,832	0.503	123	18	123	18	102	70	original
627	5 Leucine	78	Mannose	44	-0.634	-0.758	16,341	0.501	124	17	109	32	78	72	original
590	5 Leucine	41	[639; Proline (2TMS)]	45	-0.634	-0.609	17,274	0.397	125	16	88	53	90	106	original
622	5 Leucine	73	[708; Glucose methoxamine (5TMS)]	45	-0.636	-0.808	16,363	0.524	126	15	121	20	79	54	original
606	5 Leucine	57	[757; 2-Deoxy-pentose-3-yose dimethoxamine (2TMS)]	36	-0.638	-0.746	17,887	0.439	127	14	104	37	97	98	original
595	5 Leucine	46	Arabinose	45	-0.640	-0.780	19,983	0.519	128	13	114	27	107	62	original
611	5 Leucine	62	[812; D-Xylofuranose (4TMS)]	45	-0.648	-0.714	15,938	0.500	129	11	99	42	76	73	original
683	5 Leucine	134	Isomaltose	45	-0.648	-0.814	23,630	0.529	130	12	122	19	114	50	original
666	5 Leucine	117	[724; Glycerol (3TMS)]	38	-0.653	-0.884	15,620	0.549	131	10	138	3	74	38	original
635	5 Leucine	86	[793; D-Galactono-1,4-lactone (4TMS)]	45	-0.661	-0.757	24,371	0.514	132	9	107	34	116	65	original
562	5 Leucine	13	Uracil	45	-0.667	-0.878	17,541	0.582	133	8	137	4	91	23	original
659	5 Leucine	110	[715; Erythritol (4TMS)]	35	-0.677	-0.839	17,767	0.565	134	7	125	16	94	31	original
598	5 Leucine	19	Alanine (BP) (3TMS)	45	-0.681	-0.681	16,672	0.452	135	6	95	46	84	92	original
678	5 Leucine	129	[840; Maltose methoxamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	40	-0.715	-0.792	16,423	0.382	136	5	115	26	81	113	original
671	5 Leucine	122	[844; Erythritol (4TMS)]	33	-0.720	-0.887	17,881	0.522	137	4	140	1	96	58	original
599	5 Leucine	50	[746; Ribonic acid-1,4-lactone (3TMS)]	42	-0.721	-0.867	16,759	0.521	138	3	135	6	85	59	original
655	5 Leucine	106	[733; Threitol (4TMS)]	43	-0.734	-0.876	17,749	0.578	139	2	136	5	93	24	original
670	5 Leucine	121	[657; Erythritol (4TMS)]	36	-0.740	-0.885	15,335	0.502	140	1	139	2	72	71	original
770	6 Glycerol	86	[793; D-Galactono-1,4-lactone (4TMS)]	61	0.540	0.836	32,009	0.566	1	140	5	136	51	16	original
762	6 Glycerol	78	Mannose	62	0.530	0.771	44,005	0.537	2	139	9	132	109	41	original
757	6 Glycerol	73	[708; Glucose methoxamine (5TMS)]	57	0.521	0.738	41,483	0.515	3	138	17	124	97	49	original
809	6 Glycerol	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	0.512	0.895	13,908	0.554	4	137	1	140	1	27	original
760	6 Glycerol	76	Fructose	64	0.511	0.859	20,352	0.592	5	136	2	139	20	5	original
788	6 Glycerol	104	[795; Erythritol (4TMS)]	63	0.485	0.710	39,411	0.561	6	135	21	120	84	23	original
790	6 Glycerol	106	[733; Threitol (4TMS)]	62	0.492	0.769	36,780	0.596	7	134	12	129	71	3	original
724	6 Glycerol	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.477	0.624	8,064	0.504	8	133	35	106	4	54	original
723	6 Glycerol	39	[829; 1-Phenylethanol (1TMS)]	63	0.464	0.653	32,278	0.480	9	132	32	109	53	63	original

763	6	Glycerol	64	0.458	0.851	9.199	0.568	10	131	3	138	6	15	original	
703	6	Glycerol	64	0.454	0.707	32.535	0.538	11	130	23	118	54	38	original	
719	6	Glycerol	64	0.449	0.840	2.850	0.571	12	129	4	137	1	12	original	
722	6	Glycerol	64	0.448	0.828	37.061	0.470	13	128	34	107	73	66	original	
730	6	Glycerol	64	0.442	0.785	33.810	0.568	14	127	8	133	61	14	original	
708	6	Glycerol	64	0.441	0.707	12.023	0.578	15	126	22	119	7	9	original	
740	6	Glycerol	64	0.438	0.770	44.162	0.565	16	125	11	130	111	19	original	
700	6	Glycerol	64	0.436	0.665	25.764	0.553	17	124	31	110	32	28	original	
701	6	Glycerol	64	0.433	0.716	26.620	0.492	18	123	20	121	37	57	original	
697	6	Glycerol	64	0.428	0.677	28.825	0.553	19	122	27	114	42	29	original	
749	6	Glycerol	63	0.424	0.739	44.082	0.568	20	121	16	125	110	17	original	
772	6	Glycerol	64	0.415	0.667	34.760	0.522	21	120	28	113	65	46	original	
797	6	Glycerol	62	0.413	0.822	43.280	0.563	22	119	6	135	103	20	original	
713	6	Glycerol	64	0.407	0.595	40.718	0.448	23	118	40	101	93	76	original	
818	6	Glycerol	64	0.406	0.740	23.574	0.561	24	117	15	126	27	24	original	
789	6	Glycerol	62	0.393	0.818	18.148	0.534	25	116	7	134	17	42	original	
746	6	Glycerol	64	0.389	0.735	28.936	0.510	26	115	18	123	43	52	original	
698	6	Glycerol	64	0.386	0.597	46.091	0.441	27	114	38	103	114	80	original	
771	6	Glycerol	62	0.381	0.770	12.527	0.497	28	113	10	131	8	55	original	
754	6	Glycerol	57	0.377	0.668	22.917	0.485	29	112	30	111	26	59	original	
805	6	Glycerol	55	0.376	0.594	48.420	0.596	30	111	42	99	122	7	original	
801	6	Glycerol	56	0.375	0.609	40.164	0.544	31	110	37	104	90	34	original	
798	6	Glycerol	53	0.370	0.753	41.360	0.548	32	109	13	128	96	32	original	
712	6	Glycerol	64	0.368	0.582	34.518	0.452	33	108	43	98	63	72	original	
695	6	Glycerol	64	0.362	0.635	36.595	0.462	34	107	33	108	69	70	original	
734	6	Glycerol	61	0.357	0.597	55.616	0.481	35	106	39	102	137	62	original	
813	6	Glycerol	59	0.351	0.666	40.198	0.562	36	105	29	112	91	22	original	
699	6	Glycerol	64	0.348	0.701	25.505	0.545	37	104	24	117	31	33	original	
807	6	Glycerol	64	0.337	0.689	32.862	0.528	38	103	26	115	56	43	original	
705	6	Glycerol	64	0.321	0.495	26.512	0.389	39	102	47	94	36	103	original	
710	6	Glycerol	64	0.316	0.476	26.399	0.401	40	101	48	93	34	98	original	
764	6	Glycerol	62	0.314	0.752	15.605	0.511	41	100	14	127	13	51	original	
794	6	Glycerol	54	0.311	0.618	43.043	0.587	42	99	38	105	102	6	original	
706	6	Glycerol	52	0.293	0.463	45.559	0.482	43	98	51	90	112	61	original	
725	6	Glycerol	64	0.291	0.504	29.999	0.488	44	97	45	96	47	58	original	
787	6	Glycerol	63	0.286	0.502	37.334	0.466	45	96	46	95	74	69	original	
702	6	Glycerol	64	0.280	0.424	36.799	0.371	46	95	55	86	72	114	original	
804	6	Glycerol	54	0.276	0.266	29.354	0.447	47	94	64	77	48	79	original	
696	6	Glycerol	63	0.270	0.465	48.124	0.395	48	93	50	91	120	98	original	
775	6	Glycerol	64	0.263	0.408	39.640	0.449	49	92	57	84	87	73	original	
785	6	Glycerol	64	0.261	0.454	38.680	0.449	50	91	52	89	79	74	original	
741	6	Glycerol	55	0.259	0.692	35.599	0.560	51	90	25	116	68	25	original	
748	6	Glycerol	63	0.258	0.505	40.993	0.431	52	89	44	97	95	85	original	
808	6	Glycerol	52	0.252	0.449	48.580	0.554	53	88	53	88	123	26	original	
784	6	Glycerol	64	0.238	0.355	35.302	0.378	54	87	60	81	68	110	original	
786	6	Glycerol	64	0.226	0.343	42.882	0.378	55	86	61	80	100	111	original	
758	6	Glycerol	64	0.225	0.336	42.855	0.461	56	85	62	79	99	71	original	
728	6	Glycerol	50	0.221	0.429	35.491	0.622	57	84	54	87	67	2	original	
767	6	Glycerol	58	0.195	-0.059	22.606	0.314	58	83	80	61	25	135	original	
719	6	Glucose	79	Glucose	79	Glucose	79	Glucose	79	Glucose	79	Glucose	79	Glucose	
35	Pyroglutamic acid	35	Pyroglutamic acid	35	Pyroglutamic acid	35	Pyroglutamic acid	35	Pyroglutamic acid	35	Pyroglutamic acid	35	Pyroglutamic acid	35	Pyroglutamic acid
38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]
46	Arabinose	46	Arabinose	46	Arabinose	46	Arabinose	46	Arabinose	46	Arabinose	46	Arabinose	46	Arabinose
24	[725; 2-Ketooctanoic acid (2TMS)]	24	[725; 2-Ketooctanoic acid (2TMS)]	24	[725; 2-Ketooctanoic acid (2TMS)]	24	[725; 2-Ketooctanoic acid (2TMS)]	24	[725; 2-Ketooctanoic acid (2TMS)]	24	[725; 2-Ketooctanoic acid (2TMS)]	24	[725; 2-Ketooctanoic acid (2TMS)]	24	[725; 2-Ketooctanoic acid (2TMS)]
56	[829; Orotic acid (3TMS)]	56	[829; Orotic acid (3TMS)]	56	[829; Orotic acid (3TMS)]	56	[829; Orotic acid (3TMS)]	56	[829; Orotic acid (3TMS)]	56	[829; Orotic acid (3TMS)]	56	[829; Orotic acid (3TMS)]	56	[829; Orotic acid (3TMS)]
16	[644; 2-Methyl-1,3-butanediol (2TMS)]	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	16	[644; 2-Methyl-1,3-butanediol (2TMS)]
17	[700; 2-methyl-1,2-propanediol (2TMS)]	17	[700; 2-methyl-1,2-propanediol (2TMS)]	17	[700; 2-methyl-1,2-propanediol (2TMS)]	17	[700; 2-methyl-1,2-propanediol (2TMS)]	17	[700; 2-methyl-1,2-propanediol (2TMS)]	17	[700; 2-methyl-1,2-propanediol (2TMS)]	17	[700; 2-methyl-1,2-propanediol (2TMS)]	17	[700; 2-methyl-1,2-propanediol (2TMS)]
13	Uracil	13	Uracil	13	Uracil	13	Uracil	13	Uracil	13	Uracil	13	Uracil	13	Uracil
65	[646; 3-Deoxyglucitol (5TMS)]	65	[646; 3-Deoxyglucitol (5TMS)]	65	[646; 3-Deoxyglucitol (5TMS)]	65	[646; 3-Deoxyglucitol (5TMS)]	65	[646; 3-Deoxyglucitol (5TMS)]	65	[646; 3-Deoxyglucitol (5TMS)]	65	[646; 3-Deoxyglucitol (5TMS)]	65	[646; 3-Deoxyglucitol (5TMS)]
88	Gluconic acid	88	Gluconic acid	88	Gluconic acid	88	Gluconic acid	88	Gluconic acid	88	Gluconic acid	88	Gluconic acid	88	Gluconic acid
113	Galactose-6-phosphate	113	Galactose-6-phosphate	113	Galactose-6-phosphate	113	Galactose-6-phosphate	113	Galactose-6-phosphate	113	Galactose-6-phosphate	113	Galactose-6-phosphate	113	Galactose-6-phosphate
29	Erythritol	29	Erythritol	29	Erythritol	29	Erythritol	29	Erythritol	29	Erythritol	29	Erythritol	29	Erythritol
134	Isomaltose	134	Isomaltose	134	Isomaltose	134	Isomaltose	134	Isomaltose	134	Isomaltose	134	Isomaltose	134	Isomaltose
115	Glucose-6-phosphate	115	Glucose-6-phosphate	115	Glucose-6-phosphate	115	Glucose-6-phosphate	115	Glucose-6-phosphate	115	Glucose-6-phosphate	115	Glucose-6-phosphate	115	Glucose-6-phosphate
62	[812; D-Xylofuranose (4TMS)]	62	[812; D-Xylofuranose (4TMS)]	62	[812; D-Xylofuranose (4TMS)]	62	[812; D-Xylofuranose (4TMS)]	62	[812; D-Xylofuranose (4TMS)]	62	[812; D-Xylofuranose (4TMS)]	62	[812; D-Xylofuranose (4TMS)]	62	[812; D-Xylofuranose (4TMS)]
14	Fumaric acid	14	Fumaric acid	14	Fumaric acid	14	Fumaric acid	14	Fumaric acid	14	Fumaric acid	14	Fumaric acid	14	Fumaric acid
87	[945; beta-D-Glucopyranose (5TMS)]	87	[945; beta-D-Glucopyranose (5TMS)]	87	[945; beta-D-Glucopyranose (5TMS)]	87	[945; beta-D-Glucopyranose (5TMS)]	87	[945; beta-D-Glucopyranose (5TMS)]	87	[945; beta-D-Glucopyranose (5TMS)]	87	[945; beta-D-Glucopyranose (5TMS)]	87	[945; beta-D-Glucopyranose (5TMS)]
70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]
121	[657; Erythritol (4TMS)]	121	[657; Erythritol (4TMS)]	121	[657; Erythritol (4TMS)]	121	[657; Erythritol (4TMS)]	121	[657; Erythritol (4TMS)]	121	[657; Erythritol (4TMS)]	121	[657; Erythritol (4TMS)]	121	[657; Erythritol (4TMS)]
117	[724; Glycerol (3TMS)]	117	[724; Glycerol (3TMS)]	117	[724; Glycerol (3TMS)]	117	[724; Glycerol (3TMS)]	117	[724; Glycerol (3TMS)]	117	[724; Glycerol (3TMS)]	117	[724; Glycerol (3TMS)]	117	[724; Glycerol (3TMS)]
114	Fructose-6-phosphate	114	Fructose-6-phosphate	114	Fructose-6-phosphate	114	Fructose-6-phosphate	114	Fructose-6-phosphate	114	Fructose-6-phosphate	114	Fructose-6-phosphate	114	Fructose-6-phosphate
28	Malic acid	28	Malic acid	28	Malic acid	28	Malic acid	28	Malic acid	28	Malic acid	28	Malic acid	28	Malic acid
11	Succinic acid	11	Succinic acid	11	Succinic acid	11	Succinic acid	11	Succinic acid	11	Succinic acid	11	Succinic acid	11	Succinic acid
50	[748; Ribonic acid-1,4-lactone (3TMS)]	50	[748; Ribonic acid-1,4-lactone (3TMS)]	50	[748; Ribonic acid-1,4-lactone (3TMS)]	50	[748; Ribonic acid-1,4-lactone (3TMS)]	50	[748; Ribonic acid-1,4-lactone (3TMS)]	50	[748; Ribonic acid-1,4-lactone (3TMS)]	50	[748; Ribonic acid-1,4-lactone (3TMS)]	50	[748; Ribonic acid-1,4-lactone (3TMS)]
129	[840; Maltose methoxyamine (6TMS); alpha-D-Glc-(1,4)-D-Glc]	129	[840; Maltose methoxyamine (6TMS); alpha-D-Glc-(1,4)-D-Glc]	129	[840; Maltose methoxyamine (6TMS); alpha-D-Glc-(1,4)-D-Glc]	129	[840; Maltose methoxyamine (6TMS); alpha-D-Glc-(1,4)-D-Glc]	129	[840; Maltose methoxyamine (6TMS); alpha-D-Glc-(1,4)-D-Glc]	129	[840; Maltose methoxyamine (6TMS); alpha-D-Glc-(1,4)-D-Glc]	129	[840; Maltose methoxyamine (6TMS); alpha-D-Glc-(1,4)-D-Glc]	129	[840; Maltose methoxyamine (6TMS); alpha-D-Glc-(1,4)-D-Glc]
15	Alanine	15	Alanine	15	Alanine	15	Alanine	15	Alanine	15	Alanine	15	Alanine	15	Alanine
123	[945; Galactofuranose-6-phosphate (7TMS)]	123	[945; Galactofuranose-6-phosphate (7TMS)]	123	[945; Galactofuranose-6-phosphate (7TMS)]	123	[945; Galactofuranose-6-phosphate (7TMS)]	123	[945; Galactofuranose-6-phosphate (7TMS)]	123	[945; Galactofuranose-6-phosphate (7TMS)]	123	[945; Galactofuranose-6-phosphate (7TMS)]	123	[945; Galactofuranose-6-phosphate (7TMS)]
21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]
26	Citramalic acid	26	Citramalic acid	26	Citramalic acid	26	Citramalic acid	26	Citramalic acid	26	Citramalic acid	26	Citramalic acid	26	Citramalic acid
80	[772; D-Glucose (5TMS)]	80	[772; D-Glucose (5TMS)]	80	[772; D-Glucose (5TMS)]	80	[772; D-Glucose (5TMS)]	80	[772; D-Glucose (5TMS)]	80	[772; D-Glucose (5TMS)]	80	[772; D-Glucose (5TMS)]	80	[772; D-Glucose (5TMS)]
110	[715; Erythritol (4TMS)]	110	[715; Erythritol (4TMS)]	110	[715; Erythritol (4TMS)]	110	[715; Erythritol (4TMS)]	110	[715; Erythritol (4						

738	6 Glycerol	54 [NA]	55 0.195	0.594	45,588	0.537	59	82	41	100	113	40 original
763	6 Glycerol	99 [662; Ribose-5-phosphate methoxamine (BP) (5TMS)]	41 0.188	0.399	39,525	0.440	60	81	58	83	88	81 original
766	6 Glycerol	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63 0.143	0.293	54,175	0.393	61	80	63	78	136	100 original
769	6 Glycerol	85 [529; Methylenic acid (4TMS)]	48 0.137	0.215	34,575	0.307	62	79	86	75	64	138 original
780	6 Glycerol	96 myo-Inositol	49 0.134	0.107	51,669	0.258	63	78	70	71	133	138 original
819	6 Glycerol	135	64 0.102	0.114	30,974	0.347	64	77	68	73	48	130 original
776	6 Glycerol	92 [902; Melibiose (6TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	54 0.089	0.722	39,061	0.553	65	76	19	122	82	30 original
817	6 Glycerol	133 [855; Squalene]	64 0.097	0.057	39,302	0.373	66	75	74	67	83	113 original
781	6 Glycerol	97 [756; beta-D-Methylglucopyranoside (4TMS)]	52 0.094	0.424	27,944	0.563	67	74	56	85	40	21 original
816	6 Glycerol	132 [895; Isomaltose methoxamine (8TMS)]	42 0.089	0.472	43,854	0.540	68	73	49	92	107	36 original
742	6 Glycerol	58 [836; 4R-Acetamido-2,3-(Z)-epoxy-4(E)-hydroxycyclohexane (1TMS)]	64 0.080	-0.032	28,179	0.353	69	72	78	63	45	128 original
810	6 Glycerol	126 [558; Erythritol (4TMS)]	45 0.051	0.085	38,635	0.594	70	71	72	69	78	4 original
800	6 Glycerol	116 [882; Pseudouridine (5TMS)]	30 0.044	-0.140	31,507	0.194	71	70	86	55	50	140 original
793	6 Glycerol	109 Octadecanoic acid	64 0.038	0.231	26,453	0.448	72	69	65	76	35	78 original
731	6 Glycerol	47 [NA]	64 0.020	0.113	40,578	0.399	73	68	69	72	92	97 original
802	6 Glycerol	118 [928; Glucopyranose-6-phosphate (6TMS)]	58 0.018	0.384	42,217	0.434	74	67	59	82	98	83 original
10362	6 Glycerol	4 Phosphoric acid	51 0.015	-0.081	7,421	0.256	75	66	82	59	2	139 duplicate
822	6 Glycerol	138 [674; Ergosterol (1TMS)]	46 -0.001	0.012	47,226	0.357	76	65	76	65	117	126 original
814	6 Glycerol	130 Trehalose	63 -0.005	-0.102	12,984	0.361	77	64	84	57	9	124 original
9948	6 Glycerol	1 [938; Sulfuric acid (2TMS)]	36 -0.022	0.087	33,664	0.569	78	63	71	70	60	13 duplicate
778	6 Glycerol	94 Hexadecanoic acid	64 -0.025	0.079	23,747	0.527	79	62	73	68	28	45 original
759	6 Glycerol	75 Lysine	64 -0.028	-0.152	8,010	0.365	80	61	87	54	3	121 original
824	6 Glycerol	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	48 -0.043	-0.092	47,943	0.348	81	60	83	58	119	129 original
737	6 Glycerol	53 Glycerol-2-phosphate	64 -0.046	-0.175	48,279	0.355	82	59	89	52	121	127 original
795	6 Glycerol	111 [583; Erythritol (4TMS)]	42 -0.050	-0.027	51,278	0.366	83	58	77	64	131	120 original
812	6 Glycerol	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45 -0.061	0.120	32,593	0.538	84	57	67	74	55	37 original
720	6 Glycerol	36 [596; N-Acetylglutamic acid (2TMS)]	64 -0.063	-0.200	16,480	0.374	85	56	91	50	14	112 original
789	6 Glycerol	105 [705; 2-Ketogluconic acid (5TMS)]	48 -0.066	-0.073	33,851	0.566	86	55	81	60	62	18 original
782	6 Glycerol	98 [697; Ribose-5-phosphate methoxamine (5TMS)]	48 -0.099	-0.380	50,462	0.413	87	54	104	37	129	93 original
811	6 Glycerol	127 [777; Fructose-6-phosphate methoxamine (6TMS)]	39 -0.101	-0.044	33,003	0.528	88	53	79	62	57	44 original
709	6 Glycerol	25 [709; 2,5-Diaminovalerolactam (2TMS)]	48 -0.103	-0.307	43,988	0.513	89	52	98	43	108	50 original
10087	6 Glycerol	2 Serine	62 -0.112	-0.260	32,055	0.368	90	51	96	45	52	118 duplicate
755	6 Glycerol	71 [731; Erythrose (3TMS)]	64 -0.114	-0.224	31,299	0.367	91	50	93	48	49	119 original
768	6 Glycerol	84 Mannitol	62 -0.120	0.022	16,961	0.429	92	49	75	66	15	87 original
750	6 Glycerol	66 Glyceralic acid-3-phosphate	64 -0.125	-0.253	42,813	0.369	93	48	94	47	101	117 original
821	6 Glycerol	137 Ergosterol	64 -0.158	-0.254	33,058	0.364	94	46	95	46	58	122 original
707	6 Glycerol	23 Homoserine	63 -0.162	-0.452	39,490	0.414	95	47	109	32	85	92 original
756	6 Glycerol	72 [919; D-Xylopyranose (4TMS)]	53 -0.165	-0.163	43,728	0.382	96	45	88	53	105	108 original
711	6 Glycerol	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	60 -0.167	-0.400	49,290	0.360	97	44	105	38	126	125 original
777	6 Glycerol	93 [607; Putrescine (4TMS)]	60 -0.168	-0.110	52,317	0.390	98	43	85	56	135	102 original
727	6 Glycerol	43 [548; Leucine (2TBS)]	60 -0.168	-0.179	36,628	0.422	99	42	90	51	70	89 original
715	6 Glycerol	31 [622; Parabanic acid (2TMS)]	64 -0.173	-0.343	47,583	0.433	100	41	101	40	118	84 original
825	6 Glycerol	141 Lanosta-8,24-dien-3-beta-ol	61 -0.181	-0.322	50,195	0.392	101	40	100	41	128	101 original
808	6 Glycerol	124 [734; 1-Monoteoylglycerol (2TMS); 1-Monohexadecenylglycerol (1TMS)]	59 -0.186	-0.349	59,782	0.338	102	39	102	39	140	132 original
691	6 Glycerol	7 Threonine	64 -0.197	-0.302	13,352	0.385	103	38	97	44	10	106 original
692	6 Glycerol	8 Isoleucine	55 -0.205	-0.221	28,455	0.281	104	37	92	49	41	137 original
774	6 Glycerol	90 [910; 9-(Z)-Hexadecanoic acid (1TMS)]	64 -0.210	-0.418	38,285	0.425	105	36	106	35	76	88 original
693	6 Glycerol	9 Proline	63 -0.216	-0.312	25,805	0.363	106	35	99	42	33	123 original



820	6 Glycerol	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.235	-0.433	21,255	0.341	107	34	108	33	22	131 original
823	6 Glycerol	139	[700; Ergosta-5,7-dien-3-ol]	38	-0.272	-0.379	46,474	0.338	108	33	103	38	115	133 original
791	6 Glycerol	107	9-(Z)-Octadecenoic acid	64	-0.276	-0.542	29,144	0.418	109	32	117	24	44	90 original
762	6 Glycerol	68	[570; Hypoxanthine (2TMS)]	20	-0.305	-0.831	33,577	0.371	110	31	134	7	59	115 original
716	6 Glycerol	32	[729; N,N-Dimethyllysine methyl ester]	63	-0.315	-0.492	49,103	0.406	111	30	114	27	124	95 original
744	6 Glycerol	60	Glycerol-3-phosphate	64	-0.323	-0.571	22,307	0.475	112	29	120	21	24	65 original
815	6 Glycerol	131	[626; 5-Methylthioadenosine (3TMS)]	55	-0.324	-0.578	51,170	0.573	113	28	121	20	130	116 original
718	6 Glycerol	34	Aspartic acid	64	-0.326	-0.426	14,313	0.371	114	27	107	34	12	116 original
792	6 Glycerol	108	Octadecenoic acid	64	-0.336	-0.479	43,500	0.448	115	26	112	29	104	77 original
743	6 Glycerol	59	Ornithine; Arginine	64	-0.341	-0.458	8,977	0.395	116	24	110	31	5	99 original
717	6 Glycerol	61	[NA]	64	-0.341	-0.597	40,063	0.478	117	25	124	17	89	64 original
732	6 Glycerol	33	Methionine	64	-0.349	-0.494	39,767	0.381	118	23	115	26	88	109 original
714	6 Glycerol	48	Asparagine	64	-0.357	-0.747	40,845	0.542	119	22	132	9	94	35 original
751	6 Glycerol	30	[815; Ethyl-3(2H)-thiophenone]	64	-0.375	-0.463	19,409	0.387	120	21	111	30	19	104 original
721	6 Glycerol	67	Citric acid	64	-0.377	-0.600	19,190	0.468	121	20	125	16	18	67 original
803	6 Glycerol	37	Phenylalanine	64	-0.380	-0.556	20,476	0.448	122	19	118	23	21	75 original
733	6 Glycerol	119	[931; myo-Inositol-2-phosphate (7TMS)]	64	-0.381	-0.591	38,879	0.467	123	18	123	18	81	68 original
735	6 Glycerol	49	[877; Pyrophosphoric acid (4TMS)]	64	-0.392	-0.563	56,412	0.430	124	17	119	22	138	86 original
729	6 Glycerol	51	[498; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.397	-0.581	49,727	0.386	125	16	122	19	127	105 original
694	6 Glycerol	45	Homocysteine	61	-0.398	-0.518	58,438	0.416	126	15	116	25	139	91 original
753	6 Glycerol	10	Glycine	64	-0.399	-0.727	27,349	0.574	127	14	130	11	39	10 original
765	6 Glycerol	89	Arginine	60	-0.411	-0.610	26,864	0.437	128	13	127	14	38	82 original
726	6 Glycerol	81	Tyrosine	64	-0.412	-0.706	17,105	0.633	129	12	129	12	16	1 original
747	6 Glycerol	42	Glutamic acid	60	-0.415	-0.483	23,908	0.384	130	11	113	28	29	107 original
10225	6 Glycerol	63	Glutamine	52	-0.418	-0.840	43,740	0.538	131	10	135	6	106	39 original
		3	Ethanolamine	62	-0.425	-0.733	47,060	0.582	132	9	131	10	116	8 duplicate
		77	[826; beta-[(5-methyl-2-thienyl)methyleneamino- benzeneacetic acid methyl ester]	62	-0.464	-0.621	21,748	0.408	133	8	128	13	23	84 original
		55	[612; 4-Aminobutyric acid (2TBS)]	43	-0.486	-0.872	51,585	0.495	134	7	138	3	132	56 original
		5	Leucine	45	-0.501	-0.605	37,909	0.335	135	6	126	15	75	134 duplicate
		52	[NA]	46	-0.509	-0.868	49,287	0.550	136	5	137	4	125	31 original
		20		31	-0.548	-0.861	38,465	0.520	137	4	136	5	77	47 original
		89	[719; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	35	-0.563	-0.901	38,754	0.482	138	3	140	1	80	60 original
		82	Lysine	39	-0.584	-0.863	25,274	0.506	139	2	139	2	30	53 original
		95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	-0.597	-0.777	52,206	0.516	140	1	133	8	134	48 original
		9	Proline	63	0.679	0.897	14,940	0.521	1	140	1	140	29	13 original
		37	Phenylalanine	64	0.635	0.855	7,830	0.515	2	139	3	138	7	18 original
		8	Isoleucine	55	0.604	0.795	18,606	0.542	3	138	9	132	43	7 original
		2	Serine	62	0.602	0.868	20,208	0.551	4	137	2	139	49	6 duplicate
		30	[815; Ethyl-3(2H)-thiophenone]	64	0.564	0.798	8,782	0.512	5	135	7	134	8	20 original
		31	[622; Parabenic acid (2TMS)]	64	0.564	0.698	35,329	0.450	6	136	17	124	115	41 original
		33	Methionine	64	0.549	0.706	27,103	0.456	7	134	16	125	77	32 original
		60	Glycerol-3-phosphate	64	0.543	0.736	9,617	0.462	8	133	13	128	10	31 original
		66	Glyceric acid-3-phosphate	64	0.539	0.763	30,760	0.473	9	132	12	129	93	25 original
		81	Tyrosine	64	0.518	0.735	9,047	0.506	10	131	14	127	8	21 original
		32	[729; N,N-Dimethyllysine methyl ester]	63	0.510	0.799	36,590	0.525	11	130	6	135	118	11 original
		59	Ornithine; Arginine	64	0.497	0.819	11,351	0.498	12	129	5	136	16	23 original
		77	[826; beta-[(5-methyl-2-thienyl)methyleneamino- benzeneacetic acid methyl ester]	62	0.490	0.795	11,320	0.516	13	128	8	133	15	17 original
		34	Aspartic acid	64	0.478	0.696	6,262	0.445	14	127	18	123	3	45 original

885	7 Threonine	67 Citric acid	64 0.475	0.732	6.885	0.454	15	126	15	126	15	126	6	34 original
886	7 Threonine	68 [570; Hypoxanthine (2TMS)]	20 0.474	0.578	28.639	0.426	16	125	27	114	27	114	84	59 original
841	7 Threonine	23 Homoserine	64 0.464	0.548	27.053	0.448	17	124	28	113	28	113	76	43 original
10226	7 Threonine	3 Ethanolamine	62 0.463	0.639	34.909	0.455	18	123	21	120	21	120	114	33 duplicate
828	7 Threonine	10 Glycine	64 0.434	0.579	14.591	0.436	19	122	26	115	26	115	27	51 original
883	7 Threonine	75 Lysine	64 0.432	0.837	10.060	0.519	20	121	4	137	4	137	12	14 original
860	7 Threonine	42 Glutamic acid	60 0.428	0.785	14.538	0.541	21	120	10	131	10	131	25	8 original
889	7 Threonine	71 [731; Erythrose (3TMS)]	64 0.425	0.669	19.210	0.453	22	119	19	122	19	122	46	36 original
887	7 Threonine	69 Arginine	60 0.424	0.656	15.312	0.519	23	118	20	121	20	121	33	15 original
876	7 Threonine	58 [636; 4R-Acetalamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64 0.395	0.778	16.882	0.512	24	117	11	130	11	130	36	19 original
916	7 Threonine	98 [697; Ribose-5-phosphate methoxymine (5TMS)]	48 0.383	0.514	40.157	0.450	25	116	30	111	30	111	129	40 original
883	7 Threonine	45 Homocysteine	61 0.345	0.343	48.814	0.426	26	115	40	101	40	101	139	58 original
889	7 Threonine	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44 0.330	0.626	41.328	0.540	27	114	22	119	22	119	132	9 original
901	7 Threonine	83 Sorbitol	58 0.330	0.598	12.079	0.502	28	113	24	117	24	117	17	22 original
845	7 Threonine	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53 0.321	0.587	39.176	0.522	29	112	25	116	25	116	127	12 original
886	7 Threonine	48 Asparagine	64 0.307	0.417	28.236	0.408	30	111	35	106	35	106	81	76 original
879	7 Threonine	61 [NA]	64 0.285	0.321	27.831	0.361	31	110	41	100	41	100	79	109 original
10499	7 Threonine	5 Leucine	45 0.269	0.510	29.560	0.630	32	109	31	110	31	110	90	1 duplicate
934	7 Threonine	138 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17 0.265	0.525	14.552	0.286	33	108	29	112	29	112	26	134 original
854	7 Threonine	36 [596; N-Acetylglutamic acid (2TMS)]	64 0.250	0.605	5.899	0.483	34	107	23	118	23	118	2	24 original
913	7 Threonine	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50 0.231	0.301	41.800	0.315	35	106	44	97	44	97	133	132 original
956	7 Threonine	138 [674; Ergosterol (1TMS)]	46 0.229	0.385	37.506	0.365	36	105	38	103	38	103	122	104 original
882	7 Threonine	64 [788; Tyramine (3TMS)]	63 0.229	0.231	29.237	0.332	37	104	48	93	48	93	86	127 original
929	7 Threonine	111 [583; Erythritol (4TMS)]	42 0.210	0.268	40.465	0.281	38	103	46	95	46	95	130	137 original
843	7 Threonine	25 [709; 2,5-Diaminovalerolactam (2TMS)]	48 0.207	0.480	31.783	0.325	39	102	32	109	32	109	101	129 original
948	7 Threonine	130 Trehalose	63 0.198	0.446	3.334	0.391	40	101	34	107	34	107	1	87 original
942	7 Threonine	124 [734; 1-Monoolteoglycerol (2TMS); 1-Monohexadecenylglycerol (1TMS)]	59 0.197	0.344	48.297	0.349	41	100	39	102	39	102	140	116 original
833	7 Threonine	15 Alanine	64 0.192	0.137	15.175	0.414	42	99	55	88	55	88	32	72 original
955	7 Threonine	137 Ergosterol	64 0.161	0.407	21.080	0.381	43	97	38	105	38	105	50	82 original
926	7 Threonine	108 Octadecenoic acid	64 0.161	0.313	31.376	0.417	44	98	42	99	42	99	98	68 original
870	7 Threonine	52 [NA]	46 0.159	0.195	38.620	0.420	45	96	50	91	50	91	125	64 original
951	7 Threonine	133 [855; Squalene]	64 0.158	0.399	27.414	0.421	46	95	37	104	37	104	78	63 original
941	7 Threonine	123 [945; Galactofuranose-6-phosphate (7TMS)]	64 0.140	0.172	21.443	0.473	47	94	51	90	51	90	53	26 original
949	7 Threonine	131 [626; 5-Methylthiadenosine (3TMS)]	55 0.138	0.124	39.919	0.416	48	93	58	83	58	83	128	69 original
934	7 Threonine	116 [882; Pseudouridine (5TMS)]	30 0.136	0.084	24.545	0.468	49	92	59	82	59	82	62	30 original
900	7 Threonine	82 Lysine	39 0.126	0.310	17.587	0.597	50	91	43	98	43	98	40	2 original
897	7 Threonine	79 Glucose	64 0.124	-0.042	10.033	0.422	51	90	70	71	70	71	11	62 original
912	7 Threonine	94 Hexadecanoic acid	64 0.117	0.281	13.007	0.365	52	89	45	96	45	96	18	105 original
873	7 Threonine	55 [612; 4-Aminobutyric acid (2TBS)]	43 0.110	0.129	43.597	0.571	53	88	57	84	57	84	136	4 original
957	7 Threonine	139 [700; Ergosta-5,7-dien-3-ol]	38 0.110	0.154	37.576	0.341	54	87	54	87	54	87	123	121 original
907	7 Threonine	89 [775; Dopamine (4TMS)]	35 0.106	0.131	31.496	0.518	55	86	58	85	58	85	99	16 original
10363	7 Threonine	4 Phosphoric acid	51 0.101	0.461	6.526	0.526	56	85	33	108	33	108	5	10 duplicate
927	7 Threonine	109 Octadecanoic acid	64 0.100	0.244	16.987	0.339	57	84	47	94	47	94	37	124 original
861	7 Threonine	43 [548; Leucine (2TBS)]	60 0.090	0.157	25.524	0.389	58	83	53	88	53	88	68	89 original
932	7 Threonine	114 Fructose-6-phosphate	53 0.081	-0.052	30.785	0.402	59	82	72	69	72	69	94	79 original
931	7 Threonine	113 Galactose-6-phosphate	62 0.077	-0.102	32.308	0.430	60	81	76	65	76	65	104	55 original
903	7 Threonine	85 [529; Methylcitric acid (4TMS)]	48 0.073	0.072	26.048	0.566	61	80	60	81	60	81	68	5 original
914	7 Threonine	96 myo-Inositol	49 0.061	-0.032	42.519	0.396	62	79	69	72	69	72	135	85 original
887	7 Threonine	49 [877; Pyrophosphoric acid (4TMS)]	64 0.060	0.029	44.367	0.344	63	78	62	79	62	79	138	117 original

959	7 Threonine	141	Lanosta-8,24-dien-3-beta-ol	61	0.038	-0.001	38,907	0.453	64	77	65	76	126	35 original
925	7 Threonine	107	9-(Z)-Octadecenoic acid	64	0.009	0.170	17,095	0.363	65	76	52	89	38	107 original
937	7 Threonine	119	[931; myo-Inositol-2-phosphate (7TMS)]	64	-0.005	0.025	26,837	0.352	68	75	63	78	74	113 original
922	7 Threonine	104	[795; Erythritol (4TMS)]	63	-0.010	-0.011	28,520	0.442	67	74	68	73	83	47 original
920	7 Threonine	102	[904; Galactose methoxamine (5TMS)]	64	-0.015	-0.132	31,241	0.349	68	73	81	60	98	115 original
		20												
838	7 Threonine		[619; 2-(3',4'-Bishydroxyphenyl)-2-oxethylamine (4TMS)]	31	-0.015	-0.006	32,535	0.573	69	72	66	75	107	3 original
881	7 Threonine	63	Glutamine	52	-0.015	0.211	32,535	0.369	70	71	49	92	106	101 original
958	7 Threonine	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	49	-0.026	-0.074	38,467	0.419	71	70	74	67	124	65 original
944	7 Threonine	126	[559; Erythritol (4TMS)]	45	-0.042	0.056	26,673	0.339	72	69	61	80	73	123 original
		135												
953	7 Threonine		[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	-0.044	-0.079	19,237	0.334	73	68	75	68	47	126 original
853	7 Threonine	35	Pyroglutamic acid	64	-0.046	-0.241	13,137	0.400	74	67	87	54	20	81 original
837	7 Threonine	19	Alanine (BP) (3TMS)	64	-0.051	-0.049	21,730	0.396	75	66	71	70	54	84 original
859	7 Threonine	41	[839; Proline (2TMS)]	64	-0.069	0.009	18,827	0.378	76	65	64	77	45	97 original
918	7 Threonine	100	[857; Mannitol (6TMS)]	64	-0.076	-0.304	23,889	0.354	77	64	95	48	59	111 original
892	7 Threonine	74	[912; Tetradecanoic acid (1TMS)]	64	-0.077	-0.008	31,769	0.394	78	63	67	74	100	88 original
891	7 Threonine	73	[708; Glucose methoxamine (5TMS)]	57	-0.086	-0.112	32,148	0.407	79	62	78	63	103	77 original
936	7 Threonine	118	[928; Glucopyranose-6-phosphate (8TMS)]	58	-0.088	-0.108	30,948	0.317	80	61	77	64	95	131 original
933	7 Threonine	115	Glucose-6-phosphate	62	-0.102	-0.238	10,432	0.364	81	60	86	55	13	106 original
846	7 Threonine	28	Malic acid	64	-0.103	-0.383	23,216	0.449	82	59	104	37	56	42 original
836	7 Threonine	18	[590; 1-Acetyl-2-thiohydantoin]	64	-0.112	-0.053	25,274	0.366	83	58	73	68	64	103 original
862	7 Threonine	44	[910; 2-Ketogluconic acid methoxamine (4TMS)]	50	-0.117	-0.128	24,140	0.337	84	57	80	61	61	125 original
930	7 Threonine	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	-0.118	-0.202	42,514	0.374	85	56	84	57	134	98 original
950	7 Threonine	132	[895; Isomaltose methoxamine (8TMS)]	42	-0.131	-0.434	34,042	0.283	86	55	108	33	109	138 original
939	7 Threonine	121	[857; Erythritol (4TMS)]	55	-0.142	-0.132	37,096	0.324	87	54	82	59	120	130 original
908	7 Threonine	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	64	-0.152	-0.122	26,426	0.340	88	53	79	62	70	122 original
958	7 Threonine	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.155	-0.287	6,278	0.438	89	52	91	50	4	48 original
844	7 Threonine	26	Citramalic acid	64	-0.167	-0.245	14,928	0.379	90	50	88	53	31	96 original
894	7 Threonine	76	Fructose	64	-0.167	-0.314	14,777	0.380	91	51	97	44	28	95 original
928	7 Threonine	110	[715; Erythritol (4TMS)]	54	-0.177	-0.217	32,056	0.416	92	49	85	56	102	70 original
943	7 Threonine	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	-0.195	-0.331	12,888	0.372	93	48	99	42	18	99 original
896	7 Threonine	78	Mannose	62	-0.196	-0.332	33,926	0.352	94	47	100	41	108	112 original
888	7 Threonine	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	-0.197	-0.196	14,513	0.399	95	46	83	58	24	82 original
10634	7 Threonine	6	Glycerol	64	-0.197	-0.302	13,352	0.385	96	45	94	47	21	90 duplicate
832	7 Threonine	14	Fumaric acid	64	-0.200	-0.435	34,660	0.422	97	44	109	32	112	61 original
945	7 Threonine	127	[777; Fructose-6-phosphate methoxamine (6TMS)]	39	-0.201	-0.324	21,860	0.185	98	43	88	43	55	140 original
935	7 Threonine	117	[724; Glycerol (3TMS)]	56	-0.213	-0.255	29,445	0.410	99	42	89	52	89	73 original
871	7 Threonine	53	Glycerol-2-phosphate	64	-0.217	-0.294	36,511	0.343	100	41	92	49	117	119 original
890	7 Threonine	72	[918; D-Xylopyranose (4TMS)]	63	-0.218	-0.263	32,425	0.367	101	40	90	51	105	102 original
829	7 Threonine	11	Succinic acid	64	-0.224	-0.394	25,337	0.404	102	39	106	35	65	78 original
911	7 Threonine	93	[607; Putrescine (4TMS)]	60	-0.225	-0.437	41,152	0.382	103	38	110	31	131	91 original
940	7 Threonine	122	[844; Erythritol (4TMS)]	52	-0.226	-0.294	37,260	0.362	104	37	93	48	121	108 original
830	7 Threonine	12	Glyceric acid	63	-0.231	-0.467	36,646	0.381	105	36	113	28	119	94 original
924	7 Threonine	106	[733; Threitol (4TMS)]	62	-0.245	-0.313	27,036	0.442	106	35	96	45	75	46 original
839	7 Threonine	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	-0.247	-0.407	15,721	0.399	107	34	107	34	34	83 original
840	7 Threonine	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	-0.252	-0.496	35,493	0.437	108	33	115	26	116	50 original
856	7 Threonine	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.255	-0.517	26,043	0.416	109	32	117	24	67	71 original
946	7 Threonine	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	-0.277	-0.368	21,334	0.247	110	31	102	39	52	139 original
847	7 Threonine	29	Erythritol	64	-0.281	-0.552	29,307	0.446	111	30	123	18	87	44 original
898	7 Threonine	80	[772; D-Glucose (5TMS)]	62	-0.297	-0.383	13,754	0.328	112	28	103	38	22	128 original

802	7 Threonine	84	Mannitol	62	-0.306	-0.717	14,460	0.469	113	28	140	1	23	28 original	
880	7 Threonine	62	[812; D-Xylofuranosé (4TMS)]	64	-0.311	-0.461	18,046	0.381	114	27	112	29	41	93 original	
938	7 Threonine	120	[945; Uridine (3TMS)]	54	-0.314	-0.355	18,453	0.354	115	26	101	40	42	110 original	
872	7 Threonine	54	[NA]	55	-0.333	-0.498	34,521	0.344	116	23	114	27	111	118 original	
842	7 Threonine	24	[725; 2-Ketooctanoic acid (2TMS)]	64	-0.333	-0.576	10,520	0.430	117	24	127	14	14	56 original	
834	7 Threonine	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	-0.333	-0.587	16,192	0.453	118	25	130	11	35	37 original	
874	7 Threonine	56	[829; Orotic acid (3TMS)]	64	-0.336	-0.532	34,247	0.418	119	22	119	22	110	68 original	
904	7 Threonine	88	[793; D-Galactono-1,4-lactone (4TMS)]	61	-0.348	-0.496	26,581	0.469	120	21	116	25	72	29 original	
835	7 Threonine	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	-0.352	-0.545	17,490	0.431	121	20	121	20	39	54 original	
857	7 Threonine	39	[829; 1-Phenylethanol (1TMS)]	63	-0.364	-0.558	23,984	0.401	122	19	124	17	60	80 original	
909	7 Threonine	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	-0.377	-0.705	31,360	0.473	123	18	139	2	97	27 original	
919	7 Threonine	101	[832; Dopamine (4TMS)]	64	-0.379	-0.660	28,729	0.452	124	17	135	6	85	39 original	
952	7 Threonine	134	Isomaltose	64	-0.385	-0.561	18,777	0.409	125	16	125	16	44	74 original	
910	7 Threonine	92	[880; Glycerol-2-phosphata (4TMS)]	54	-0.385	-0.391	28,070	0.292	126	15	105	36	80	133 original	
906	7 Threonine	88	Gluconic acid	64	-0.390	-0.578	25,124	0.436	127	14	128	13	63	52 original	
921	7 Threonine	103	[848; Ethylamine (2TMS)]	63	-0.398	-0.643	28,439	0.434	128	13	133	8	82	53 original	
831	7 Threonine	13	Uracil	64	-0.403	-0.603	19,779	0.453	129	12	132	9	48	38 original	
864	7 Threonine	46	Arabinose	64	-0.406	-0.544	26,320	0.417	130	11	120	21	69	67 original	
905	7 Threonine	87	[945; beta-D-Glucopyranose (5TMS)]	62	-0.435	-0.445	14,918	0.389	131	10	111	30	30	88 original	
875	7 Threonine	57	[757; 2-Desoxy-pentos-3-ylose dimethoxyamine (2TMS)]	55	-0.438	-0.524	26,535	0.342	132	9	118	23	71	120 original	
883	7 Threonine	65	[846; 3-Deoxyglucitol (5TMS)]	63	-0.439	-0.546	34,814	0.408	133	8	122	19	113	75 original	
865	7 Threonine	47	[NA]	64	-0.457	-0.569	30,018	0.426	134	7	126	15	91	60 original	
947	7 Threonine	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	-0.465	-0.583	30,563	0.370	135	6	129	12	92	100 original	
915	7 Threonine	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	-0.481	-0.686	21,185	0.426	136	5	137	4	51	57 original	
868	7 Threonine	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	-0.484	-0.650	44,334	0.438	137	4	134	7	137	49 original	
923	7 Threonine	105	[705; 2-Ketogluconic acid (5TMS)]	48	-0.491	-0.682	23,443	0.349	138	3	136	5	57	114 original	
917	7 Threonine	99	[862; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	-0.529	-0.596	29,316	0.272	139	2	131	10	88	138 original	
9949	7 Threonine	1	[938; Sulfuric acid (2TMS)]	36	-0.568	-0.699	23,486	0.284	140	1	138	3	58	135 duplicate	
960	8 Isoleucine	9	Proline	54	0.883	0.978	11,789	0.648	140	1	140	1	140	8	1 original
1019	8 Isoleucine	68	[570; Hypoxanthine (2TMS)]	18	0.752	0.539	19,998	0.434	2	139	28	112	69	39 original	
984	8 Isoleucine	33	Methionine	55	0.732	0.534	13,523	0.488	3	138	31	110	16	19 original	
981	8 Isoleucine	30	[815; Ethyl-3(2H)-thiophenone]	55	0.719	0.608	17,712	0.534	4	137	20	121	52	12 original	
982	8 Isoleucine	31	[822; Parabanic acid (2TMS)]	55	0.717	0.707	20,111	0.451	5	136	13	128	72	34 original	
0089	8 Isoleucine	2	Serine	55	0.700	0.930	5,391	0.558	6	135	2	139	1	3 duplicate	
974	8 Isoleucine	23	Homoserine	55	0.667	0.521	13,808	0.473	7	134	32	109	18	23 original	
0500	8 Isoleucine	5	Leucine	45	0.616	0.861	19,616	0.545	8	133	3	138	65	7 duplicate	
0769	8 Isoleucine	7	Threonine	55	0.604	0.795	18,608	0.542	9	132	4	137	62	9 duplicate	
985	8 Isoleucine	34	Aspartic acid	55	0.600	0.500	20,550	0.467	10	131	34	107	77	27 original	
961	8 Isoleucine	10	Glycine	55	0.595	0.564	10,871	0.353	11	130	25	116	5	85 original	
1010	8 Isoleucine	59	Ornithine; Arginine	55	0.593	0.727	27,626	0.537	12	129	10	131	127	11 original	
1020	8 Isoleucine	69	Arginine	55	0.589	0.634	11,038	0.433	13	128	19	122	7	40 original	
983	8 Isoleucine	32	[729; N,N-Dimethyllysine methyl ester]	55	0.580	0.737	17,774	0.484	14	127	9	132	53	21 original	
1032	8 Isoleucine	81	Tyrosine	55	0.576	0.693	20,749	0.461	15	126	14	127	80	30 original	
993	8 Isoleucine	42	Glutamic acid	54	0.561	0.765	15,708	0.507	16	125	6	135	32	15 original	
1017	8 Isoleucine	66	Glyceric acid-3-phosphate	55	0.546	0.721	17,338	0.514	17	124	12	129	49	14 original	
1028	8 Isoleucine	77	[826; beta-[[[5-methyl-2-thienyl)methylethylamino- benzeneacetic acid methyl ester]	54	0.537	0.746	16,720	0.519	18	123	8	133	43	13 original	
996	8 Isoleucine	45	Homocysteine	52	0.523	0.196	31,478	0.412	19	122	51	90	137	44 original	
1002	8 Isoleucine	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	41	0.520	0.537	29,462	0.545	20	121	30	111	134	8 original	

988	8 Isoleucine	37 Phenylalanine	55 0.518	0.689	13.439	0.455	21	120	15	128	15	32 original
976	8 Isoleucine	25 [708; 2,5-Diaminovalerolactam (2TMS)]	39 0.511	0.509	16.736	0.404	22	119	33	108	44	47 original
999	8 Isoleucine	48 Asparagine	55 0.495	0.394	15.662	0.351	23	118	39	102	30	87 original
10227	8 Isoleucine	3 Ethanolamine	54 0.480	0.580	19.752	0.437	24	117	24	117	68	36 duplicate
978	8 Isoleucine	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	49 0.466	0.583	23.816	0.495	25	116	23	118	103	18 original
1040	8 Isoleucine	89 [775; Dopamine (4TMS)]	34 0.451	0.288	21.788	0.459	26	115	45	98	84	31 original
1049	8 Isoleucine	98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	42 0.449	0.401	25.788	0.436	27	114	38	103	118	37 original
1033	8 Isoleucine	82 Lysine	39 0.433	0.673	10.972	0.501	28	113	17	124	6	16 original
1006	8 Isoleucine	55 [612; 4-Aminobutyric acid (2TBS)]	43 0.393	0.391	33.449	0.470	29	112	40	101	140	25 original
1012	8 Isoleucine	61 [NA]	55 0.380	0.138	16.890	0.302	30	111	55	86	45	121 original
1000	8 Isoleucine	49 [877; Pyrophosphoric acid (4TMS)]	55 0.347	0.270	29.485	0.340	31	110	46	95	135	97 original
1018	8 Isoleucine	67 Citric acid	55 0.345	0.545	14.554	0.412	32	109	28	113	22	45 original
1026	8 Isoleucine	75 Lysine	55 0.344	0.788	26.529	0.558	33	108	5	136	124	4 original
994	8 Isoleucine	43 [548; Leucine (2TBS)]	52 0.306	0.200	15.415	0.345	34	107	50	91	29	91 original
1011	8 Isoleucine	60 Glycerol-3-phosphate	55 0.298	0.590	12.603	0.484	35	106	22	119	12	20 original
1082	8 Isoleucine	131 [626; 5-Methylthiadenosine (3TMS)]	47 0.295	0.217	26.369	0.360	36	105	49	92	121	75 original
1087	8 Isoleucine	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17 0.284	0.559	6.337	0.187	37	104	26	115	2	138 original
1009	8 Isoleucine	58 [636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	55 0.292	0.721	10.222	0.556	38	103	11	130	4	5 original
1003	8 Isoleucine	52 [NA]	37 0.267	0.173	25.315	0.404	39	102	52	89	112	49 original
1059	8 Isoleucine	108 Octadecenoic acid	55 0.235	0.434	18.391	0.343	40	101	37	104	60	94 original
1046	8 Isoleucine	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	42 0.233	0.300	27.755	0.380	41	100	43	98	128	65 original
971	8 Isoleucine	20 [819; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31 0.230	0.548	24.308	0.466	42	99	27	114	107	28 original
1014	8 Isoleucine	63 Glutamine	43 0.192	0.231	20.445	0.261	43	98	48	93	75	133 original
987	8 Isoleucine	124 [734; 1-Monodecylglycerol (2TMS); 1-Monohexadecylglycerol (1TMS)]	55 0.162	0.752	16.345	0.540	44	97	7	134	37	10 original
1075	8 Isoleucine	15 Alanine	51 0.107	0.591	32.297	0.356	45	96	21	120	139	79 original
966	8 Isoleucine	71 [731; Erythrose (3TMS)]	55 0.091	0.019	14.457	0.387	46	95	62	79	21	62 original
1022	8 Isoleucine	130 Trehalose	55 0.086	0.329	12.456	0.453	47	94	42	99	11	33 original
1081	8 Isoleucine	107 9-(Z)-Octadecenoic acid	54 0.068	0.290	18.661	0.364	48	93	44	97	63	73 original
1058	8 Isoleucine	4 Phosphoric acid	55 0.055	0.659	17.359	0.548	50	91	18	123	50	103 original
10364	8 Isoleucine	79 Glucose	55 0.053	-0.032	23.440	0.416	51	90	66	75	100	42 original
1030	8 Isoleucine	64 [789; Tyramine (3TMS)]	54 0.043	-0.016	17.980	0.283	52	89	64	77	58	126 original
1015	8 Isoleucine	93 [607; Putrescine (4TMS)]	51 0.024	-0.336	29.103	0.477	53	88	100	41	133	22 original
1044	8 Isoleucine	53 Glycerol-2-phosphate	55 -0.020	-0.091	23.717	0.325	54	87	68	73	101	109 original
1004	8 Isoleucine	137 Ergosterol	55 -0.021	0.438	11.996	0.380	55	86	38	105	9	66 original
1088	8 Isoleucine	119 [931; myo-Inositol-2-phosphate (7TMS)]	55 -0.029	0.089	18.669	0.345	56	85	58	83	41	90 original
1070	8 Isoleucine	111 [583; Erythritol (4TMS)]	36 -0.032	0.157	26.846	0.231	57	84	54	87	125	134 original
1062	8 Isoleucine	83 Sorbitol	52 -0.051	0.682	8.193	0.587	58	83	16	125	3	2 original
1034	8 Isoleucine	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	55 -0.056	-0.007	16.667	0.338	59	82	63	78	40	100 original
1041	8 Isoleucine	133 [855; Squalene]	39 -0.093	0.457	15.316	0.414	60	81	35	106	28	43 original
1084	8 Isoleucine	138 [674; Ergosterol (1TMS)]	53 -0.123	-0.753	22.786	0.461	62	79	139	2	92	29 original
1035	8 Isoleucine	141 Lanosta-8,24-dien-3-beta-ol	31 -0.139	0.135	25.471	0.380	63	78	56	85	114	67 original
1090	8 Isoleucine	139 [700; Ergosta-5,7-dien-3-ol]	55 -0.145	0.022	25.504	0.350	64	77	61	80	115	88 original
1060	8 Isoleucine	109 Octadecanoic acid	55 -0.162	0.123	17.247	0.331	65	76	57	94	47	106 original
1053	8 Isoleucine	102 [904; Galactose methoxyamine (5TMS)]	55 -0.170	-0.236	20.031	0.320	66	75	79	62	70	113 original
1045	8 Isoleucine	94 Hexadecanoic acid	46 -0.175	0.165	14.833	0.320	67	74	53	88	24	114 original
1047	8 Isoleucine	96 myo-Inositol		-0.160	30.288	0.297	68	73	73	68	136	123 original

1074	8 Isoleucine	123 [945; Galactofuranose-6-phosphate (7TMS)]	55 -0.177	0.038	13.927	0.403	69	71	59	82	19	50 original
1023	8 Isoleucine	72 [919; D-Xylopyranose (4TMS)]	55 -0.177	-0.241	21.868	0.334	70	72	80	61	85	104 original
1069	8 Isoleucine	118 [928; Glucopyranose-6-phosphate (6TMS)]	49 -0.190	-0.054	19.946	0.276	71	70	67	74	67	130 original
1055	8 Isoleucine	104 [795; Erythritol (4TMS)]	55 -0.196	0.026	17.884	0.404	72	69	60	81	56	48 original
1064	8 Isoleucine	113 Galactose-6-phosphate	53 -0.200	-0.170	21.618	0.371	73	68	75	66	82	72 original
10635	8 Isoleucine	6 Glycerol	55 -0.205	-0.221	28.455	0.281	74	67	78	63	131	127 duplicate
1051	8 Isoleucine	100 [857; Mannitol (6TMS)]	55 -0.208	-0.331	16.065	0.338	75	66	97	44	35	89 original
1065	8 Isoleucine	114 Fructose-6-phosphate	44 -0.214	-0.137	20.068	0.305	76	65	70	71	71	119 original
135												
1086	8 Isoleucine	126 [559; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	55 -0.223	-0.336	13.557	0.355	77	64	89	42	17	82 original
1077	8 Isoleucine	126 [559; Erythritol (4TMS)]	36 -0.235	-0.030	16.623	0.388	78	63	65	76	39	61 original
1042	8 Isoleucine	91 [766; beta-D-Methylglucopyranoside (4TMS)]	55 -0.254	-0.691	26.975	0.472	79	62	138	3	126	24 original
1067	8 Isoleucine	116 [882; Pseudouridine (5TMS)]	30 -0.255	-0.302	16.925	0.399	80	61	88	53	46	53 original
1083	8 Isoleucine	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	54 -0.259	-0.328	28.549	0.353	81	60	96	45	132	86 original
998	8 Isoleucine	47 [NA]	55 -0.263	-0.429	22.418	0.356	82	59	105	36	88	80 original
986	8 Isoleucine	35 Pyroglutamic acid	55 -0.266	-0.311	28.332	0.330	83	58	89	52	130	108 original
1036	8 Isoleucine	85 [529; Methylcitric acid (4TMS)]	48 -0.270	-0.436	15.884	0.496	84	57	107	34	33	17 original
1071	8 Isoleucine	120 [945; Uridine (3TMS)]	45 -0.287	-0.322	14.849	0.306	85	56	94	47	25	118 original
995	8 Isoleucine	44 [910; 2-Ketogluconic acid methoxamine (4TMS)]	41 -0.293	-0.191	17.844	0.298	86	55	76	65	54	122 original
1078	8 Isoleucine	127 [777; Fructose-6-phosphate methoxamine (8TMS)]	30 -0.297	-0.274	14.692	0.061	87	54	82	59	23	140 original
1091	8 Isoleucine	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	42 -0.298	-0.150	26.403	0.428	88	53	72	69	122	41 original
1025	8 Isoleucine	74 [912; Tetradecanoic acid (1TMS)]	55 -0.300	-0.165	21.913	0.393	89	52	74	67	86	57 original
1066	8 Isoleucine	115 Glucose-6-phosphate	53 -0.300	-0.279	17.959	0.287	90	51	84	57	57	125 original
1024	8 Isoleucine	73 [708; Glucose methoxamine (5TMS)]	51 -0.316	-0.286	21.707	0.450	91	50	86	55	83	35 original
963	8 Isoleucine	12 Glycic acid	54 -0.317	-0.556	24.951	0.360	92	49	121	20	110	76 original
979	8 Isoleucine	28 Malic acid	55 -0.328	-0.479	16.027	0.398	93	47	110	31	34	55 original
989	8 Isoleucine	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	55 -0.329	-0.534	18.185	0.345	94	48	117	24	59	92 original
1031	8 Isoleucine	80 [772; D-Glucose (5TMS)]	53 -0.331	-0.289	22.832	0.277	95	46	87	54	95	129 original
1027	8 Isoleucine	76 Fructose	55 -0.333	-0.334	20.632	0.339	96	44	98	43	79	98 original
1079	8 Isoleucine	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	36 -0.333	-0.364	16.345	0.174	97	45	104	37	36	138 original
991	8 Isoleucine	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	55 -0.335	-0.321	22.451	0.409	98	41	92	49	89	46 original
1076	8 Isoleucine	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	55 -0.335	-0.342	23.269	0.313	99	42	101	40	99	116 original
1052	8 Isoleucine	101 [832; Dopamine (4TMS)]	55 -0.335	-0.665	22.531	0.469	100	43	136	5	91	26 original
1083	8 Isoleucine	132 [895; Isomaltose methoxamine (8TMS)]	33 -0.348	-0.436	25.272	0.127	101	40	106	35	111	139 original
1029	8 Isoleucine	78 Mannose	53 -0.356	-0.320	23.822	0.344	102	39	91	50	104	93 original
980	8 Isoleucine	29 Erythritol	55 -0.356	-0.602	19.359	0.360	103	38	131	10	64	58 original
969	8 Isoleucine	18 [590; 1-Acetyl-2-thiohydantoin]	55 -0.370	-0.282	16.576	0.340	104	37	85	58	38	96 original
970	8 Isoleucine	19 Alanine (BP) (3TMS)	55 -0.375	-0.534	17.318	0.322	105	36	71	70	31	111 original
962	8 Isoleucine	11 Succinic acid	55 -0.382	-0.534	17.318	0.373	106	35	118	23	48	69 original
1061	8 Isoleucine	110 [715; Erythritol (4TMS)]	45 -0.386	-0.261	23.141	0.382	107	34	81	60	97	64 original
965	8 Isoleucine	14 Fumaric acid	55 -0.390	-0.505	23.178	0.394	108	33	111	30	98	56 original
1048	8 Isoleucine	97 [756; beta-D-Methylglucopyranoside (4TMS)]	43 -0.391	-0.633	22.811	0.401	109	32	134	7	83	52 original
1068	8 Isoleucine	117 [724; Glycerol (3TMS)]	47 -0.393	-0.278	20.516	0.372	110	31	83	58	76	70 original
1072	8 Isoleucine	121 [657; Erythritol (4TMS)]	46 -0.401	-0.214	24.874	0.312	111	30	77	64	109	117 original
1054	8 Isoleucine	103 [648; Ethylamine (2TMS)]	54 -0.405	-0.648	24.192	0.435	112	29	135	6	106	38 original
1021	8 Isoleucine	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	51 -0.412	-0.322	12.909	0.384	113	28	93	48	13	63 original
992	8 Isoleucine	41 [639; Proline (2TMS)]	55 -0.414	-0.131	14.280	0.320	114	25	89	72	20	115 original
975	8 Isoleucine	24 [725; 2-Ketooctanoic acid (2TMS)]	55 -0.414	-0.591	22.528	0.355	115	26	129	12	90	81 original
967	8 Isoleucine	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	55 -0.414	-0.621	16.682	0.379	116	27	133	8	42	68 original
968	8 Isoleucine	17 [700; 2-methyl-1,2-propanediol (2TMS)]	55 -0.420	-0.557	17.566	0.358	117	24	122	19	51	77 original
1057	8 Isoleucine	106 [733; Threitol (4TMS)]	53 -0.427	-0.324	20.442	0.401	118	23	95	46	74	51 original

1039	8 Isoleucine	88	Gluconic acid	55	-0.433	-0.523	19,949	0.371	119	22	115	26	68	71 original
1038	8 Isoleucine	127	[945; beta-D-Glucopyranose (5TMS)]	54	-0.434	-0.363	25,535	0.305	120	21	103	38	116	120 original
1073	8 Isoleucine	182	[644; Erythritol (4TMS)]	43	-0.435	-0.317	26,522	0.358	121	20	80	51	123	78 original
1043	8 Isoleucine	92	[680; Glycerol-2-phosphate (4TMS)]	45	-0.438	-0.344	20,305	0.224	122	18	102	39	73	135 original
1037	8 Isoleucine	86	[793; D-Galactono-1,4-lactone (4TMS)]	54	-0.440	-0.468	26,246	0.355	123	18	109	32	120	84 original
972	8 Isoleucine	21	[678; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	55	-0.440	-0.515	14,927	0.399	124	17	113	28	27	54 original
1007	8 Isoleucine	56	[829; Orotic acid (3TMS)]	55	-0.446	-0.566	26,237	0.338	125	16	124	17	119	101 original
977	8 Isoleucine	26	Citramalic acid	55	-0.449	-0.461	13,404	0.388	126	15	108	33	14	60 original
990	8 Isoleucine	39	[829; 1-Phenylethanol (1TMS)]	54	-0.458	-0.572	22,074	0.337	127	14	126	15	87	102 original
997	8 Isoleucine	46	Arabinose	55	-0.461	-0.532	24,041	0.331	128	13	116	25	105	107 original
1085	8 Isoleucine	134	Isomaltose	55	-0.476	-0.555	22,815	0.341	129	12	120	21	94	95 original
1005	8 Isoleucine	54	[NA]	46	-0.492	-0.578	25,539	0.280	130	11	128	13	117	128 original
1016	8 Isoleucine	65	[646; 3-Deoxyglucitol (5TMS)]	54	-0.497	-0.542	27,843	0.323	131	10	119	22	129	110 original
973	8 Isoleucine	21	[690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	45	-0.505	-0.513	25,447	0.322	132	9	112	29	113	112 original
964	8 Isoleucine	13	Uracil	55	-0.508	-0.611	18,566	0.363	133	8	132	9	61	74 original
1008	8 Isoleucine	57												
1013	8 Isoleucine		[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	46	-0.509	-0.515	23,024	0.268	134	7	114	27	96	131 original
1056	8 Isoleucine		[812; D-Xylofuranose (4TMS)]	55	-0.522	-0.561	14,923	0.347	135	6	123	18	26	89 original
			[705; 2-Ketogluconic acid (5TMS)]	39	-0.522	-0.668	20,631	0.332	136	5	137	4	78	105 original
			[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-O-Glc]											
1080	8 Isoleucine	50	[746; Ribonic acid-1,4-lactone (3TMS)]	50	-0.546	-0.566	24,503	0.290	137	4	125	16	108	124 original
1001	8 Isoleucine	52	[746; Ribonic acid-1,4-lactone (3TMS)]	52	-0.557	-0.602	31,632	0.355	138	3	130	11	138	83 original
1050	8 Isoleucine	32	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	32	-0.569	-0.577	21,016	0.186	139	2	127	14	81	137 original
9950	8 Isoleucine	1	[938; Sulfuric acid (2TMS)]	27	-0.601	-0.755	17,862	0.264	140	1	140	1	55	132 duplicate
10803	9 Proline	8	Isoleucine	54	0.883	0.978	11,789	0.648	1	140	1	140	9	1 duplicate
10090	9 Proline	2	Serine	61	0.809	0.965	10,969	0.599	2	139	2	139	3	4 duplicate
1114	9 Proline	31	[822; Parabanic acid (2TMS)]	63	0.747	0.763	30,371	0.478	3	138	15	128	99	34 original
1116	9 Proline	33	Methionine	63	0.732	0.718	21,833	0.454	4	137	19	122	42	43 original
1113	9 Proline	30	[815; Ethyl-3(2H)-thiophenone]	63	0.731	0.795	11,070	0.511	5	136	11	130	8	22 original
10770	9 Proline	7	Threonine	63	0.679	0.897	14,840	0.521	6	134	3	138	17	19 duplicate
1106	9 Proline	23	Homoserine	63	0.679	0.646	22,153	0.505	7	135	29	112	44	24 original
1115	9 Proline	32	[729; N,N-Dimethyllysine methyl ester]	62	0.855	0.869	28,788	0.558	8	133	6	135	92	12 original
1151	9 Proline	68	[570; Hypoxanthine (2TMS)]	20	0.653	0.667	28,103	0.430	9	132	28	113	71	67 original
1142	9 Proline	59	Ornithine; Arginine	63	0.849	0.856	21,000	0.511	10	131	9	132	38	21 original
1117	9 Proline	34	Aspartic acid	63	0.832	0.704	14,892	0.442	11	130	22	119	18	54 original
1164	9 Proline	81	Tyrosine	63	0.821	0.793	13,869	0.519	12	129	12	129	14	20 original
1149	9 Proline	66	Glycic acid-3-phosphate	63	0.617	0.791	26,922	0.496	13	128	13	128	77	28 original
1093	9 Proline	10	Glycine	63	0.597	0.680	13,319	0.432	14	127	26	115	11	65 original
1152	9 Proline	69	Arginine	59	0.596	0.727	11,015	0.549	15	126	17	124	5	14 original
1125	9 Proline	42	Glutamic acid	59	0.594	0.868	8,001	0.563	16	125	7	134	1	10 original
1110	9 Proline	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	52	0.575	0.709	33,981	0.537	17	124	21	120	120	17 original
10501	9 Proline	5	Leucine	45	0.574	0.874	28,751	0.637	18	123	5	136	90	2 duplicate
			[826; beta-[(S-methyl-2-thienyl)methyleneamino-benzeneacetic acid methyl ester]											
1160	9 Proline	37	Phenylalanine	61	0.573	0.860	8,809	0.544	19	122	8	133	2	15 original
1120	9 Proline	63	0.559	63	0.559	0.811	13,731	0.483	20	121	10	131	13	31 original
1181	9 Proline	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	47	0.530	0.547	35,251	0.465	21	120	34	107	125	38 original
10228	9 Proline	3	Ethanolamine	61	0.525	0.704	29,871	0.470	22	119	24	117	98	37 duplicate
1158	9 Proline	75	Lysine	63	0.520	0.891	20,006	0.535	23	118	4	137	31	18 original
1128	9 Proline	45	Homocysteine	60	0.512	0.386	41,994	0.417	24	117	42	99	138	78 original
1134	9 Proline	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	0.490	0.718	39,674	0.586	25	116	18	123	135	7 original

1141	9 Proline	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	63	0.479	0.788	14.123	0.501	26	115	14	127	15	28 original
1131	9 Proline	48	Asparagine	63	0.448	0.488	23.837	0.442	27	114	36	105	55	55 original
1172	9 Proline	89	[775; Dopamine (4TMS)]	34	0.437	0.401	28.956	0.579	28	113	41	100	93	9 original
1165	9 Proline	82	Lysine	39	0.414	0.732	15.714	0.569	29	112	16	125	18	6 original
1150	9 Proline	67	Citric acid	63	0.413	0.689	14.572	0.418	30	111	25	116	16	77 original
1108	9 Proline	25	[709; 2,5-Diaminovalerolactam (2TMS)]	47	0.406	0.595	24.182	0.427	31	110	32	109	58	71 original
1143	9 Proline	60	Glycerol-3-phosphate	63	0.389	0.679	13.616	0.507	32	109	27	114	12	23 original
1219	9 Proline	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	16	0.333	0.630	11.160	0.377	33	108	31	110	7	102 original
1144	9 Proline	61	[NA]	63	0.314	0.224	25.589	0.344	34	107	49	92	66	123 original
1138	9 Proline	55	[612; 4-Aminobutyric acid (2TBS)]	43	0.307	0.410	43.123	0.594	35	106	40	101	140	5 original
1119	9 Proline	36	[596; N-Acetylglutamic acid (2TMS)]	63	0.296	0.715	13.044	0.542	36	105	20	121	10	18 original
1178	9 Proline	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	49	0.281	0.425	37.922	0.328	37	104	39	102	131	131 original
1126	9 Proline	43	[548; Leucine (2TBS)]	60	0.273	0.234	23.712	0.387	38	103	48	93	52	94 original
1214	9 Proline	131	[626; 5-Methylthioadenosine (3TMS)]	54	0.254	0.213	36.047	0.441	39	102	50	91	129	56 original
1213	9 Proline	130	Trehalose	62	0.249	0.475	16.358	0.376	40	101	37	104	20	107 original
1132	9 Proline	49	[877; Pyrophosphoric acid (4TMS)]	63	0.242	0.166	39.670	0.342	41	100	53	88	134	124 original
1154	9 Proline	71	[731; Erythrose (3TMS)]	63	0.228	0.591	18.911	0.444	42	99	33	108	28	52 original
10365	9 Proline	4	Phosphoric acid	51	0.225	0.704	11.579	0.559	43	98	23	118	8	11 duplicate
1103	9 Proline	20		31	0.183	0.531	32.218	0.582	44	97	35	106	110	8 original
1135	9 Proline	52	[NA]	45	0.172	0.199	33.457	0.428	45	96	51	90	116	69 original
1191	9 Proline	108	Octadecanoic acid	63	0.157	0.337	27.934	0.372	46	95	44	97	84	111 original
1098	9 Proline	15	Alanine	63	0.139	0.058	18.103	0.441	47	94	60	81	23	58 original
1162	9 Proline	79	Glucose	63	0.125	-0.090	21.736	0.462	48	93	67	74	41	40 original
1207	9 Proline	124	[734; 1-Monooctadecylglycerol (2TMS); 1-Monohexadecylglycerol (1TMS)]	58	0.122	0.469	42.982	0.368	49	92	38	103	139	112 original
1147	9 Proline	64	[789; Tyramine (3TMS)]	62	0.117	0.081	26.825	0.319	50	91	58	83	75	133 original
1168	9 Proline	83	Sorbitol	57	0.112	0.645	11.002	0.555	51	90	30	111	4	13 original
1146	9 Proline	63	Glutamine	51	0.106	0.282	27.253	0.353	52	89	46	95	79	120 original
1221	9 Proline	138	[674; Ergosterol (1TMS)]	45	0.028	0.261	32.818	0.374	53	88	47	94	112	110 original
1194	9 Proline	111	[583; Erythritol (4TMS)]	41	0.000	0.059	35.429	0.305	54	87	59	82	126	134 original
1216	9 Proline	133	[655; Squalene]	63	-0.011	0.342	24.474	0.398	55	85	43	98	60	85 original
1220	9 Proline	137	Ergosterol	63	-0.011	0.323	19.122	0.381	56	86	45	96	27	98 original
1222	9 Proline	139	[700; Ergosta-5,7-dien-3-ol]	38	-0.021	0.108	33.507	0.273	57	84	55	88	117	137 original
1208	9 Proline	123	[945; Galactofuranose-6-phosphate (7TMS)]	63	-0.041	0.090	21.077	0.433	58	83	57	84	39	64 original
1201	9 Proline	118	[928; Glucopyranose-6-phosphate (6TMS)]	57	-0.045	-0.020	28.154	0.324	59	82	65	76	87	132 original
1190	9 Proline	107	9-(Z)-Octadecenoic acid	63	-0.050	0.095	18.425	0.337	60	81	58	85	25	127 original
1202	9 Proline	119	[931; myo-Inositol-2-phosphate (7TMS)]	63	-0.069	-0.011	25.236	0.375	61	80	63	78	63	109 original
1187	9 Proline	104	[795; Erythritol (4TMS)]	62	-0.084	0.010	26.643	0.433	62	79	61	80	74	63 original
1155	9 Proline	72	[919; D-Xylopyranose (4TMS)]	62	-0.114	-0.160	30.440	0.376	63	78	69	72	103	106 original
1177	9 Proline	94	Hexadecanoic acid	63	-0.115	0.169	16.903	0.331	64	77	52	89	21	130 original
1197	9 Proline	114	Fructose-6-phosphate	52	-0.118	-0.173	27.826	0.377	65	76	71	70	83	103 original
1196	9 Proline	113	Galactose-6-phosphate	61	-0.122	-0.223	30.325	0.410	66	75	79	62	87	82 original
1209	9 Proline	126	[559; Erythritol (4TMS)]	44	-0.123	0.008	23.002	0.419	67	74	62	79	47	76 original
1224	9 Proline	141	Lanosta-8,24-dien-3-beta-ol	61	-0.129	-0.020	35.861	0.394	68	73	64	77	128	87 original
1192	9 Proline	109	Octadecanoic acid	63	-0.131	0.139	19.381	0.332	69	72	54	87	28	129 original
1136	9 Proline	53	Glycerol-2-phosphate	63	-0.137	-0.241	33.415	0.349	70	71	80	61	114	121 original
1179	9 Proline	96	myo-Inositol	49	-0.160	-0.178	39.783	0.377	71	70	72	69	136	104 original
1173	9 Proline	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	63	-0.188	-0.209	25.304	0.347	72	69	75	66	64	122 original
1176	9 Proline	93	[607; Putrescine (4TMS)]	60	-0.198	-0.420	38.531	0.415	73	68	95	46	132	79 original



10636	9 Proline	6	Glycerol	63	-0.216	-0.312	25.805	0.363	74	67	84	57	67	116 duplicate
1223	9 Proline	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	49	-0.219	-0.140	35.600	0.384	75	66	68	73	127	96 original
1118	9 Proline	35	Pyroglutamic acid	63	-0.221	-0.374	25.884	0.392	76	65	91	50	70	88 original
1124	9 Proline	41	[639; Proline (2TMS)]	63	-0.235	-0.075	20.105	0.398	77	64	68	75	32	86 original
1199	9 Proline	116	[882; Pseudouridine (5TMS)]	30	-0.241	-0.392	23.933	0.503	78	63	93	48	56	25 original
1210	9 Proline	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	38	-0.246	-0.356	19.465	0.156	79	62	87	54	29	140 original
1185	9 Proline	102	[904; Galactose methoxyamine (5TMS)]	63	-0.248	-0.354	28.220	0.376	80	61	88	55	94	108 original
1102	9 Proline	19	Alanine (BP) (3TMS)	63	-0.247	-0.169	22.444	0.365	81	60	70	71	46	115 original
1127	9 Proline	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	49	-0.250	-0.219	23.439	0.356	82	59	77	64	50	119 original
1156	9 Proline	73	[708; Glucose methoxyamine (5TMS)]	56	-0.262	-0.220	31.416	0.490	83	58	78	63	105	30 original
1168	9 Proline	85	[528; Malic acid (4TMS)]	48	-0.270	-0.529	25.844	0.603	84	57	107	34	68	3 original
1163	9 Proline	80	[772; D-Glucose (5TMS)]	61	-0.272	-0.358	23.752	0.335	85	56	88	53	53	128 original
135														
1218	9 Proline		[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	63	-0.283	-0.349	20.237	0.359	86	55	85	56	34	118 original
1198	9 Proline	115	Glucose-6-phosphate	61	-0.294	-0.368	19.756	0.402	87	54	90	51	30	84 original
1183	9 Proline	100	[857; Mannitol (6TMS)]	63	-0.294	-0.463	24.006	0.378	88	53	102	39	57	101 original
1204	9 Proline	121	[657; Erythritol (4TMS)]	54	-0.297	-0.217	33.621	0.342	89	52	76	65	118	126 original
1215	9 Proline	132	[895; Isomaltose methoxyamine (8TMS)]	41	-0.302	-0.555	31.576	0.242	90	51	108	33	106	139 original
1159	9 Proline	76	Fructose	63	-0.305	-0.413	23.271	0.379	91	50	94	47	49	99 original
1193	9 Proline	110	[715; Erythritol (4TMS)]	53	-0.306	-0.289	30.406	0.452	92	49	82	59	102	45 original
1157	9 Proline	74	[912; Tetradecanoic acid (1TMS)]	63	-0.308	-0.204	30.388	0.410	93	48	74	67	101	80 original
1130	9 Proline	47	[NA]	63	-0.321	-0.502	30.380	0.424	94	47	106	35	100	73 original
1200	9 Proline	117	[724; Glycerol (3TMS)]	55	-0.325	-0.305	28.043	0.379	96	45	83	58	86	100 original
1111	9 Proline	28	Malic acid	63	-0.332	-0.577	23.705	0.436	97	44	109	32	51	60 original
1123	9 Proline	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	63	-0.336	-0.436	20.419	0.460	98	43	99	42	36	42 original
1161	9 Proline	78	Mannose	61	-0.354	-0.435	33.167	0.368	99	42	97	44	113	113 original
1211	9 Proline	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	44	-0.355	-0.480	21.579	0.260	100	41	105	36	40	138 original
1205	9 Proline	122	[644; Erythritol (4TMS)]	51	-0.357	-0.364	34.510	0.392	101	40	89	52	122	89 original
1203	9 Proline	120	[945; Uridine (3TMS)]	53	-0.357	-0.431	20.394	0.391	102	39	96	45	35	91 original
1101	9 Proline	18	[590; 1-Acetyl-2-thiohydantoin]	63	-0.358	-0.265	24.573	0.367	103	38	81	60	61	114 original
1195	9 Proline	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	62	-0.363	-0.466	38.703	0.390	104	37	103	38	133	92 original
1208	9 Proline	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	63	-0.368	-0.436	24.301	0.392	105	36	98	43	59	90 original
1174	9 Proline	91	[766; beta-D-Methylglucopyranoside (4TMS)]	63	-0.380	-0.751	35.144	0.493	106	35	137	4	124	29 original
1189	9 Proline	106	[733; Threitol (4TMS)]	61	-0.383	-0.382	27.676	0.472	107	34	92	49	81	36 original
1153	9 Proline	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	56	-0.392	-0.188	17.530	0.431	108	33	73	68	22	68 original
1184	9 Proline	101	[832; Dopamine (4TMS)]	63	-0.399	-0.700	30.365	0.461	109	32	128	13	98	41 original
1121	9 Proline	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	63	-0.401	-0.660	26.367	0.434	110	31	121	20	73	61 original
1097	9 Proline	26	Citramalic acid	63	-0.405	-0.474	18.329	0.410	111	30	104	37	24	81 original
1094	9 Proline	14	Fumaric acid	63	-0.416	-0.625	32.574	0.437	112	29	115	26	111	59 original
1170	9 Proline	11	Succinic acid	63	-0.420	-0.606	25.372	0.429	113	28	112	29	65	68 original
1112	9 Proline	87	[945; beta-D-Glucopyranose (5TMS)]	61	-0.444	-0.463	25.878	0.384	114	27	101	40	69	97 original
1095	9 Proline	29	Erythritol	63	-0.444	-0.713	28.177	0.481	115	26	132	9	88	33 original
1186	9 Proline	12	Glyceric acid	62	-0.457	-0.677	34.372	0.441	116	25	124	17	121	57 original
1104	9 Proline	103	[648; Ethylamine (2TMS)]	62	-0.478	-0.709	31.676	0.464	117	24	131	10	108	39 original
1139	9 Proline	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	63	-0.481	-0.618	20.164	0.448	118	23	113	28	33	51 original
1100	9 Proline	56	[828; Orotic acid (3TMS)]	63	-0.482	-0.849	34.684	0.433	119	22	116	25	123	62 original
1169	9 Proline	17	[700; 2-methyl-1,2-propanediol (2TMS)]	63	-0.493	-0.659	23.112	0.449	120	21	120	21	48	48 original
1107	9 Proline	86	[793; D-Galactono-1,4-lactone (4TMS)]	60	-0.494	-0.597	31.669	0.452	121	20	110	31	107	46 original
		24	[725; 2-Ketocacetic acid (2TMS)]	63	-0.494	-0.706	23.820	0.449	122	19	129	12	54	50 original
		22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	51	-0.495	-0.652	33.778	0.443	123	18	117	24	119	53 original

1099	9 Proline	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	63	-0.495	-0.728	22,073	0.474	124	17	134	7	43	35 original
1180	9 Proline	97	[756; beta-D-Methylglucopyranoside (4TMS)]	51	-0.504	-0.709	28,255	0.451	125	16	130	11	89	47 original
1145	9 Proline	62	[812; D-Xylofuranose (4TMS)]	63	-0.508	-0.605	20,897	0.404	128	15	111	30	37	83 original
1175	9 Proline	92	[680; Glycerol-2-phosphate (4TMS)]	53	-0.512	-0.442	27,449	0.303	127	14	100	41	80	135 original
1217	9 Proline	134	Isomaltose	63	-0.519	-0.674	27,804	0.427	128	13	123	18	82	70 original
1122	9 Proline	39	[829; 1-Phenylethanol (1TMS)]	62	-0.525	-0.683	28,781	0.421	129	12	126	15	91	74 original
1129	9 Proline	46	Arabinose	63	-0.532	-0.653	31,088	0.428	130	11	118	23	104	72 original
1096	9 Proline	13	Uracil	63	-0.557	-0.722	24,934	0.453	131	10	133	8	62	44 original
1171	9 Proline	88	Gluconic acid	63	-0.561	-0.758	28,042	0.481	132	9	138	3	85	32 original
57														
1140	9 Proline	54	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	54	-0.563	-0.622	29,399	0.362	133	7	114	27	95	117 original
1137	9 Proline	54	[NA]	54	-0.563	-0.664	33,415	0.387	134	8	122	19	115	93 original
9951	9 Proline	1	[938; Sulfuric acid (2TMS)]	35	-0.563	-0.769	22,193	0.342	135	6	139	2	45	125 duplicate
1148	9 Proline	65	[646; 3-Deoxyglucitol (5TMS)]	62	-0.567	-0.659	36,109	0.420	136	5	119	22	130	75 original
1212	9 Proline	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	58	-0.575	-0.679	32,174	0.386	137	4	125	16	109	95 original
1182	9 Proline	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	40	-0.595	-0.692	26,899	0.298	138	3	127	14	76	136 original
1133	9 Proline	50	[746; Ribonic acid-1,4-lactone (3TMS)]	60	-0.598	-0.737	41,340	0.449	139	2	135	6	137	49 original
1188	9 Proline	105	[705; 2-Ketogluconic acid (5TMS)]	47	-0.604	-0.739	26,192	0.377	140	1	136	5	72	105 original
1295	10 Glycine	81	Tyrosine	64	0.781	0.903	16,198	0.658	1	140	4	137	50	25 original
10502	10 Glycine	5	Leucine	45	0.772	0.858	19,255	0.558	2	139	13	128	66	71 duplicate
1265	10 Glycine	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	0.751	0.861	31,774	0.552	3	138	12	129	134	74 original
10229	10 Glycine	3	Ethanolamine	62	0.748	0.891	22,141	0.630	4	137	8	133	89	35 duplicate
1282	10 Glycine	68	[570; Hypoxanthine (2TMS)]	20	0.747	0.949	23,590	0.616	5	138	2	139	100	44 original
1291	10 Glycine	77	[826; beta-[(5-methyl-2-thienyl)methyleneamino-benzeneacetic acid methyl ester]	62	0.746	0.839	12,632	0.508	6	135	14	127	22	91 original
1256	10 Glycine	42	Glutamic acid	60	0.728	0.791	13,704	0.461	7	134	18	123	31	113 original
1296	10 Glycine	82	Lysine	39	0.727	0.856	7,486	0.701	8	133	1	140	4	7 original
1269	10 Glycine	55	[812; 4-Aminobutyric acid (2TBS)]	43	0.721	0.872	34,165	0.592	9	132	10	131	138	57 original
1282	10 Glycine	48	Asparagine	64	0.687	0.892	14,434	0.669	10	131	7	134	35	16 original
1283	10 Glycine	69	Arginine	60	0.678	0.896	5,682	0.620	11	130	8	135	2	41 original
1244	10 Glycine	30	[815; Ethyl-3(2H)-thiophenone]	64	0.677	0.715	13,312	0.447	12	129	25	116	27	117 original
1273	10 Glycine	59	Ornithine; Arginine	64	0.675	0.757	24,257	0.502	13	128	20	121	104	83 original
1303	10 Glycine	89	[775; Dopamine (4TMS)]	35	0.630	0.886	21,464	0.605	14	127	9	132	85	47 original
1247	10 Glycine	33	Methionine	64	0.625	0.697	14,774	0.512	15	126	26	115	38	89 original
1246	10 Glycine	32	[728; N,N-Dimethyllysine methyl ester]	63	0.623	0.834	23,432	0.598	16	125	15	128	97	50 original
20														
1234	10 Glycine	9	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	0.600	0.907	25,647	0.672	17	124	3	138	110	15 original
11036	10 Glycine	9	Proline	63	0.597	0.680	13,319	0.432	18	123	29	112	28	124 duplicate
1345	10 Glycine	131	[626; 5-Methylthiadenosine (3TMS)]	55	0.596	0.745	28,287	0.630	19	122	21	120	126	34 original
10804	10 Glycine	8	Isoleucine	55	0.595	0.564	10,871	0.353	20	121	38	103	14	137 duplicate
1251	10 Glycine	37	Phenylalanine	64	0.594	0.743	8,146	0.500	21	120	22	119	5	94 original
1309	10 Glycine	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	0.587	0.720	31,927	0.540	22	119	24	117	135	79 original
1245	10 Glycine	31	[622; Parabenic acid (2TMS)]	64	0.583	0.766	22,737	0.533	23	118	19	122	91	81 original
1281	10 Glycine	67	Citric acid	64	0.550	0.680	9,378	0.477	24	117	28	113	8	103 original
1248	10 Glycine	34	Aspartic acid	64	0.537	0.645	16,373	0.489	25	116	30	111	53	98 original
1259	10 Glycine	45	Homocysteine	61	0.528	0.639	34,600	0.463	26	115	32	109	139	112 original
1237	10 Glycine	23	Homoserine	64	0.527	0.862	13,706	0.597	27	114	11	130	32	51 original
1274	10 Glycine	60	Glycerol-3-phosphate	64	0.508	0.622	7,364	0.523	28	113	34	107	3	85 original
1280	10 Glycine	66	Glyceric acid-3-phosphate	64	0.478	0.686	18,726	0.524	29	112	27	114	63	84 original
10081	10 Glycine	2	Serine	62	0.469	0.615	11,572	0.440	30	111	35	108	16	119 duplicate

1263	10 Glycine	49	[877; Pyrophosphoric acid (4TMS)]	64	0.459	0.628	31,065	0.483	31	110	33	108	133	101 original
1275	10 Glycine	61	[NA]	64	0.450	0.561	16,098	0.516	32	109	39	102	49	88 original
1239	10 Glycine	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	0.450	0.898	18,204	0.633	33	107	5	138	62	32 original
1312	10 Glycine	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	68	0.450	0.795	29,814	0.567	34	108	17	124	131	67 original
10771	10 Glycine	7	Threonine	64	0.434	0.579	14,591	0.438	35	106	37	104	36	122 duplicate
1241	10 Glycine	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	0.421	0.830	27,264	0.591	36	105	16	125	120	58 original
1289	10 Glycine	75	Lysine	64	0.393	0.555	23,459	0.455	37	104	40	101	98	115 original
1250	10 Glycine	36	[596; N-Acetylglutamic acid (2TMS)]	64	0.370	0.587	12,826	0.438	38	103	68	105	24	121 original
1266	10 Glycine	52	[NA]	46	0.362	0.644	28,376	0.665	39	102	31	110	127	21 original
1322	10 Glycine	108	Octadecanoic acid	64	0.328	0.496	19,305	0.414	40	101	41	100	68	128 original
1257	10 Glycine	43	[548; Leucine (2TBS)]	60	0.272	0.464	14,405	0.488	41	100	42	99	34	98 original
		58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	0.261	0.445	8,883	0.390	42	99	43	98	7	133 original
1272	10 Glycine	71	[731; Erythrose (3TMS)]	64	0.235	0.285	9,753	0.471	43	98	47	94	11	107 original
1285	10 Glycine	63	Glutamine	52	0.228	0.737	20,018	0.679	44	97	23	118	72	12 original
1344	10 Glycine	130	Trehalose	63	0.215	0.314	15,054	0.400	45	96	46	95	40	132 original
10368	10 Glycine	4	Phosphoric acid	51	0.176	0.378	17,530	0.337	46	95	44	97	57	139 duplicate
		124	[734; 1-Monoocteoxyglycerol (2TMS); 1-Monohexadecenoxyglycerol (1TMS)]	59	0.172	0.316	38,423	0.404	47	94	45	96	140	131 original
1338	10 Glycine	107	9-(Z)-Octadecanoic acid	64	0.115	0.281	8,530	0.409	48	93	49	92	6	129 original
1321	10 Glycine	119	[931; myo-Inositol-2-phosphate (7TMS)]	64	0.097	0.151	15,923	0.516	49	92	51	90	46	87 original
1333	10 Glycine	137	Ergosterol	64	0.072	0.168	12,788	0.470	50	91	50	91	23	109 original
1351	10 Glycine	138	[748; D-Scdheptulose-7-phosphate (7TMS)]	17	0.029	-0.002	5,182	0.456	51	90	55	85	1	114 original
1350	10 Glycine	72	[918; D-Xylopyranose (4TMS)]	63	-0.009	0.029	21,178	0.339	52	89	55	86	82	138 original
1286	10 Glycine	53	Glycerol-2-phosphate	64	-0.012	0.051	24,623	0.385	53	88	53	88	106	135 original
1267	10 Glycine	64	[789; Tyramine (3TMS)]	63	-0.015	-0.188	18,178	0.472	54	87	60	81	61	106 original
1278	10 Glycine	15	Alanine	64	-0.021	-0.332	12,422	0.667	55	86	69	72	19	19 original
1308	10 Glycine	94	Hexadecanoic acid	64	-0.033	-0.272	13,484	0.476	56	85	65	76	30	104 original
1352	10 Glycine	138	[674; Ergosterol (1TMS)]	46	-0.036	-0.099	21,177	0.452	57	84	59	82	119	116 original
1304	10 Glycine	90	[910; 9-(Z)-Hexadecanoic acid (1TMS)]	64	-0.038	0.058	15,554	0.438	58	83	52	89	42	120 original
1355	10 Glycine	141	Larosta-8,24-dien-3-beta-ol	61	-0.040	-0.079	27,688	0.483	59	82	58	83	123	102 original
1323	10 Glycine	108	Octadecanoic acid	64	-0.									

1316	10	Glycine	102	[904; Galactose methoxyamine (5TMS)]	64	-0.319	-0.556	20.503	0.543	79	62	78	63	75	77	original
1322	10	Glycine	18	[590; 1-Acetyl-2-thiohydantoin]	64	-0.337	-0.535	15.745	0.468	80	61	76	65	45	110	original
1288	10	Glycine	74	[912; Tetradecanoic acid (1TMS)]	64	-0.340	-0.607	23.301	0.485	81	60	82	59	96	99	original
1326	10	Glycine	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	-0.350	-0.628	30.759	0.507	82	59	83	58	132	92	original
1255	10	Glycine	41	[639; Proline (2TMS)]	64	-0.350	-0.560	12.568	0.496	83	58	79	62	20	95	original
1289	10	Glycine	85	[529; Methylcitric acid (4TMS)]	48	-0.351	-0.646	17.584	0.468	84	57	86	55	58	111	original
1330	10	Glycine	116	[882; Pseudouridine (5TMS)]	30	-0.356	-0.317	17.830	0.445	85	56	67	74	60	118	original
1258	10	Glycine	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	-0.357	-0.721	15.978	0.667	86	55	92	49	47	20	original
1314	10	Glycine	100	[857; Mannitol (6TMS)]	64	-0.369	-0.662	14.837	0.542	87	54	88	53	39	78	original
1313	10	Glycine	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	-0.368	-0.853	19.851	0.612	88	53	114	27	70	45	original
9852	10	Glycine	1	[938; Sulfuric acid (2TMS)]	36	-0.394	-0.649	13.380	0.624	89	52	87	54	29	37	duplicate
1233	10	Glycine	19	Alanine (BP) (3TMS)	64	-0.397	-0.685	15.234	0.544	90	51	89	52	41	76	original
10637	10	Glycine	6	Glycerol	64	-0.399	-0.727	27.349	0.574	91	50	94	47	121	65	duplicate
1334	10	Glycine	120	[945; Uridine (3TMS)]	54	-0.400	-0.320	10.870	0.623	92	49	68	73	13	38	original
1342	10	Glycine	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	-0.408	-0.750	12.614	0.622	93	48	97	44	21	39	original
1346	10	Glycine	132	[895; Isomaltose methoxyamine (8TMS)]	42	-0.429	-0.912	25.040	0.640	94	47	127	14	108	29	original
1305	10	Glycine	81	[766; beta-D-Methylglucopyranoside (4TMS)]	64	-0.438	-0.643	25.650	0.484	95	46	84	57	111	100	original
1331	10	Glycine	117	[724; Glycerol (3TMS)]	56	-0.439	-0.767	20.753	0.587	96	45	101	40	78	60	original
1336	10	Glycine	122	[644; Erythritol (4TMS)]	52	-0.449	-0.828	27.037	0.596	97	44	112	29	118	52	original
1311	10	Glycine	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	-0.454	-0.757	20.598	0.561	98	43	99	42	76	69	original
1324	10	Glycine	110	[715; Erythritol (4TMS)]	54	-0.455	-0.821	23.512	0.669	99	42	108	33	99	17	original
1335	10	Glycine	121	[657; Erythritol (4TMS)]	55	-0.465	-0.732	26.602	0.594	100	41	98	45	118	55	original
1294	10	Glycine	80	[772; D-Glucose (5TMS)]	62	-0.480	-0.728	21.913	0.512	101	40	95	46	88	33	original
1249	10	Glycine	35	Pyroglutamic acid	64	-0.485	-0.854	27.350	0.630	102	39	115	26	122	88	original
1329	10	Glycine	115	Glucose-6-phosphate	62	-0.491	-0.840	16.233	0.641	103	38	113	28	51	28	original
1319	10	Glycine	105	[705; 2-Ketogluconic acid (5TMS)]	48	-0.498	-0.790	16.057	0.605	104	37	104	37	48	48	original
1235	10	Glycine	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	-0.508	-0.818	25.728	0.576	105	36	98	43	17	64	original
1226	10	Glycine	12	Glyceric acid	63	-0.508	-0.818	25.728	0.576	106	35	107	34	113	66	original
1315	10	Glycine	101	[832; Dopamine (4TMS)]	64	-0.511	-0.703	21.088	0.531	107	34	90	51	80	83	original
1240	10	Glycine	26	Citramalic acid	64	-0.513	-0.781	9.594	0.552	108	33	102	39	9	73	original
1254	10	Glycine	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.529	-0.808	19.998	0.596	109	32	106	35	71	53	original
1292	10	Glycine	73	[708; Glucose methoxyamine (5TMS)]	62	-0.529	-0.824	25.726	0.580	110	31	110	31	112	62	original
1287	10	Glycine	78	Mannose	57	-0.530	-0.758	24.636	0.537	111	30	100	41	107	80	original
1339	10	Glycine	125	[892; Sucrose (6TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	-0.540	-0.826	22.745	0.639	112	29	111	30	92	30	original
1290	10	Glycine	76	Fructose	64	-0.545	-0.888	20.074	0.678	113	28	118	23	73	13	original
1308	10	Glycine	92	[680; Glycerol-2-phosphate (4TMS)]	54	-0.551	-0.794	19.053	0.585	114	27	105	36	64	61	original
1284	10	Glycine	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	-0.553	-0.601	13.281	0.531	115	26	81	60	26	82	original
1317	10	Glycine	103	[648; Ethylamine (2TMS)]	63	-0.560	-0.789	22.979	0.565	116	25	103	38	94	68	original
1320	10	Glycine	106	[733; Threitol (4TMS)]	62	-0.571	-0.854	20.810	0.710	117	24	116	25	79	31	original
1242	10	Glycine	28	Malic acid	64	-0.578	-0.903	14.862	0.638	118	23	123	18	37	6	original
1301	10	Glycine	87	[945; beta-D-Glucopyranose (5TMS)]	62	-0.590	-0.823	25.568	0.551	119	22	109	32	109	75	original
1243	10	Glycine	29	Erythritol	64	-0.593	-0.888	19.076	0.629	120	21	119	22	65	36	original
1252	10	Glycine	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.607	-0.923	17.383	0.662	121	20	128	13	56	22	original
1225	10	Glycine	11	Succinic acid	64	-0.620	-0.864	16.284	0.594	122	19	117	24	52	54	original
1253	10	Glycine	39	[828; 1-Phenylethanol (1TMS)]	63	-0.623	-0.933	21.260	0.659	123	18	130	11	83	24	original
1228	10	Glycine	14	Fumaric acid	64	-0.626	-0.908	24.027	0.620	124	17	126	15	102	40	original
1302	10	Glycine	88	Glutaric acid	64	-0.653	-0.905	19.432	0.668	125	16	124	17	69	18	original
1266	10	Glycine	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	-0.653	-0.900	25.730	0.619	126	15	122	19	114	42	original
1231	10	Glycine	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	-0.655	-0.893	15.588	0.609	127	14	120	21	43	46	original
1276	10	Glycine	62	[812; D-Xylofuranose (4TMS)]	64	-0.657	-0.900	12.171	0.646	128	13	121	20	18	27	original

1343	10 Glycine	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	-0.667	-0.948	23,929	0.873	129	12	133	8	101	14 original
1230	10 Glycine	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	-0.672	-0.934	14,300	0.891	130	11	131	10	33	10 original
1268	10 Glycine	54	[NA]	55	-0.879	-0.906	24,560	0.588	131	10	125	16	105	59 original
1270	10 Glycine	56	[829; Orolic acid (3TMS)]	64	-0.681	-0.956	26,528	0.701	132	9	136	5	115	8 original
1238	10 Glycine	24	[725; 2-Ketooctanoic acid (2TMS)]	64	-0.684	-0.955	21,428	0.713	133	8	135	6	84	2 original
1348	10 Glycine	134	Isomaltose	64	-0.689	-0.966	22,757	0.720	134	7	140	1	93	1 original
1271	10 Glycine	57	[757; 2-Desoxy-pentose-3-ylose dimethoxyamine (2TMS)]	55	-0.694	-0.944	21,636	0.687	135	6	132	9	86	11 original
1260	10 Glycine	46	Arabinose	64	-0.700	-0.958	24,112	0.712	136	5	138	3	103	3 original
1264	10 Glycine	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	-0.706	-0.931	33,200	0.604	137	3	129	12	137	49 original
1300	10 Glycine	86	[793; D-Galactono-1,4-lactone (4TMS)]	61	-0.706	-0.949	26,872	0.712	138	4	134	7	117	4 original
1279	10 Glycine	65	[646; 3-Deoxyglucitol (5TMS)]	63	-0.731	-0.961	28,200	0.711	139	2	139	2	125	5 original
1227	10 Glycine	13	Uracil	64	-0.737	-0.957	17,100	0.698	140	1	137	4	54	9 original
1360	11 Succinic acid	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	0.800	0.934	11,615	0.630	1	140	2	139	58	4 original
1368	11 Succinic acid	24	[725; 2-Ketooctanoic acid (2TMS)]	64	0.798	0.929	26,407	0.614	2	139	4	137	127	13 original
1358	11 Succinic acid	14	Fumaric acid	64	0.782	0.926	9,627	0.633	3	138	5	136	39	3 original
1373	11 Succinic acid	29	Erythritol	64	0.779	0.940	4,369	0.650	4	137	1	140	7	1 original
1356	11 Succinic acid	12	Glycic acid	63	0.752	0.892	11,874	0.585	5	136	16	125	59	30 original
1382	11 Succinic acid	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.743	0.931	1,915	0.630	6	135	3	138	1	5 original
1372	11 Succinic acid	28	Malic acid	64	0.736	0.919	2,576	0.604	7	134	6	135	2	21 original
1398	11 Succinic acid	55	[700; 2-methyl-1,2-propanediol (2TMS)]	55	0.723	0.896	12,528	0.605	8	133	13	128	64	20 original
1361	11 Succinic acid	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	0.713	0.895	11,534	0.592	9	132	14	127	55	26 original
1357	11 Succinic acid	13	Uracil	64	0.712	0.907	10,230	0.611	10	131	8	133	44	16 original
1406	11 Succinic acid	62	[812; D-Xylofuranose (4TMS)]	64	0.711	0.877	7,873	0.611	11	130	20	121	25	17 original
1390	11 Succinic acid	46	Arabinose	64	0.707	0.904	13,063	0.627	12	129	10	131	68	7 original
1409	11 Succinic acid	65	[646; 3-Deoxyglucitol (5TMS)]	63	0.704	0.914	12,737	0.621	13	128	7	134	68	9 original
1401	11 Succinic acid	57	[757; 2-Desoxy-pentose-3-ylose dimethoxyamine (2TMS)]	55	0.702	0.891	10,985	0.617	14	127	17	124	51	11 original
1400	11 Succinic acid	56	[829; Orolic acid (3TMS)]	64	0.695	0.906	10,524	0.627	15	126	9	132	46	6 original
1383	11 Succinic acid	39	[829; 1-Phenylethanol (1TMS)]	63	0.685	0.897	11,284	0.612	16	125	12	129	54	15 original
1430	11 Succinic acid	86	[793; D-Galactono-1,4-lactone (4TMS)]	61	0.684	0.893	17,655	0.624	17	124	15	128	90	8 original
1478	11 Succinic acid	134	Isomaltose	64	0.683	0.904	19,519	0.616	18	123	11	130	106	12 original
1473	11 Succinic acid	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	0.674	0.889	10,144	0.559	19	122	18	123	43	41 original
1366	11 Succinic acid	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.667	0.887	13,124	0.607	20	121	19	122	69	19 original
1432	11 Succinic acid	88	Gluconic acid	64	0.658	0.854	7,093	0.571	21	120	24	117	19	35 original
1394	11 Succinic acid	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	0.647	0.861	20,087	0.570	22	119	22	119	108	36 original
1365	11 Succinic acid	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	0.636	0.832	10,537	0.541	23	118	30	111	47	52 original
1370	11 Succinic acid	26	Citramalic acid	64	0.621	0.835	10,593	0.553	24	117	28	113	48	43 original
1384	11 Succinic acid	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.605	0.835	29,248	0.613	25	116	26	115	132	14 original
1459	11 Succinic acid	115	Glucose-6-phosphate	62	0.602	0.833	16,892	0.590	26	115	29	112	102	27 original
1420	11 Succinic acid	76	Fructose	64	0.585	0.836	19,851	0.567	27	114	25	116	107	39 original
1469	11 Succinic acid	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	0.578	0.778	26,353	0.563	28	113	32	109	126	44 original
1378	11 Succinic acid	35	Pyrogallamic acid	64	0.575	0.835	35,983	0.550	29	112	27	114	138	45 original
1456	11 Succinic acid	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.558	0.775	18,141	0.503	30	111	33	108	96	65 original
1414	11 Succinic acid	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	0.554	0.563	13,451	0.431	31	110	60	81	72	100 original
1417	11 Succinic acid	73	[708; Glucose methoxyamine (5TMS)]	57	0.549	0.754	9,723	0.473	32	109	35	106	40	75 original
1422	11 Succinic acid	78	Mannose	62	0.546	0.766	10,761	0.493	33	108	34	107	49	71 original
1447	11 Succinic acid	103	[648; Ethylamine (2TMS)]	63	0.543	0.741	11,164	0.516	34	107	39	102	53	59 original
1436	11 Succinic acid	92	[680; Glycerol-2-phosphate (4TMS)]	54	0.533	0.712	8,161	0.498	35	106	43	98	26	69 original

1464	11 Succinic acid	120 [945; Uridine (3TMS)]	54	0.525	0.386	6.628	0.594	36	105	71	70	15	25 original
1450	11 Succinic acid	106 [733; Threitol (4TMS)]	62	0.519	0.788	7.497	0.608	37	104	31	110	23	18 original
1443	11 Succinic acid	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	0.515	0.868	11.613	0.847	38	103	21	120	57	2 original
1444	11 Succinic acid	100 [657; Mannitol (6TMS)]	64	0.513	0.754	2.974	0.504	39	102	36	105	3	64 original
1446	11 Succinic acid	102 [904; Galactose methoxyamine (5TMS)]	64	0.509	0.726	6.759	0.501	40	101	40	101	18	67 original
1479	11 Succinic acid	135	64	0.488	0.672	6.483	0.463	41	100	48	93	13	82 original
1476	11 Succinic acid	132 [895; Isomaltose methoxyamine (8TMS)]	42	0.487	0.859	16.553	0.597	42	99	23	116	81	23 original
1460	11 Succinic acid	116 [882; Pseudouridine (5TMS)]	30	0.487	0.477	8.711	0.310	43	98	64	77	32	139 original
1445	11 Succinic acid	101 [832; Dopamine (4TMS)]	64	0.456	0.642	8.335	0.474	44	97	53	88	29	74 original
1465	11 Succinic acid	121 [657; Erythritol (4TMS)]	55	0.453	0.693	15.161	0.544	45	96	45	96	76	50 original
1362	11 Succinic acid	18 [590; 1-Acetyl-2-thiohydantoin]	64	0.451	0.669	3.071	0.449	46	95	49	92	4	88 original
1449	11 Succinic acid	105 [705; 2-Ketogluconic acid (5TMS)]	48	0.447	0.673	9.578	0.531	47	94	47	94	37	57 original
1441	11 Succinic acid	97 [756; beta-D-Methylglucopyranoside (4TMS)]	52	0.439	0.660	16.645	0.511	48	93	51	90	82	61 original
1461	11 Succinic acid	117 [724; Glycerol (3TMS)]	56	0.438	0.682	8.610	0.535	49	92	46	95	30	54 original
1429	11 Succinic acid	85 [529; Methylenic acid (4TMS)]	48	0.436	0.664	3.158	0.447	50	91	50	91	5	91 original
1435	11 Succinic acid	91 [766; beta-D-Methylglucopyranoside (4TMS)]	64	0.411	0.605	14.922	0.436	51	90	57	84	75	86 original
1472	11 Succinic acid	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.406	0.749	5.637	0.555	52	89	37	104	8	42 original
1454	11 Succinic acid	110 [715; Erythritol (4TMS)]	54	0.406	0.716	12.315	0.568	53	88	42	99	62	38 original
1457	11 Succinic acid	113 Galactose-6-phosphate	62	0.402	0.742	8.858	0.521	54	87	38	103	33	58 original
1466	11 Succinic acid	122 [644; Erythritol (4TMS)]	52	0.397	0.723	16.988	0.532	55	86	41	100	87	56 original
1458	11 Succinic acid	114 Fructose-6-phosphate	53	0.377	0.711	9.555	0.534	56	85	44	97	36	55 original
9953	11 Succinic acid	1 Fructose-6-phosphate	36	0.371	0.482	9.033	0.574	57	84	66	75	34	31 duplicate
1363	11 Succinic acid	19 Alanine (BP) (3TMS)	64	0.370	0.618	6.636	0.448	58	83	55	86	16	90 original
10638	11 Succinic acid	8 Glycerol	64	0.362	0.635	36.595	0.462	59	82	54	87	140	84 duplicate
1418	11 Succinic acid	74 [912; Tetradecanoic acid (1TMS)]	64	0.353	0.576	9.789	0.465	60	81	58	83	41	80 original
1431	11 Succinic acid	87 [945; beta-D-Glucopyranose (5TMS)]	62	0.352	0.609	30.079	0.447	61	80	56	85	135	82 original
1388	11 Succinic acid	44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	0.334	0.645	8.241	0.550	62	79	52	89	27	46 original
1470	11 Succinic acid	126 [559; Erythritol (4TMS)]	45	0.305	0.523	9.408	0.569	63	78	61	80	35	37 original
1385	11 Succinic acid	41 [639; Proline (2TMS)]	64	0.278	0.454	8.306	0.409	64	77	67	74	28	112 original
1440	11 Succinic acid	96 myo-Inositol	49	0.277	0.273	20.284	0.300	65	76	75	66	109	140 original
1471	11 Succinic acid	127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.263	0.563	6.022	0.586	66	75	59	82	12	28 original
1427	11 Succinic acid	83 Sorbitol	58	0.261	-0.261	17.357	0.367	67	74	93	48	89	132 original
1448	11 Succinic acid	104 [795; Erythritol (4TMS)]	63	0.245	0.409	6.753	0.435	68	73	70	71	17	98 original
1467	11 Succinic acid	123 [945; Galactofuranose-6-phosphate (7TMS)]	64	0.235	0.440	5.598	0.455	69	72	68	73	8	86 original
1455	11 Succinic acid	111 [583; Erythritol (4TMS)]	42	0.231	0.424	21.661	0.423	70	71	69	72	114	104 original
1426	11 Succinic acid	84 Mannitol	62	0.219	0.471	26.821	0.432	71	70	65	76	128	99 original
1424	11 Succinic acid	80 [772; D-Glucose (5TMS)]	62	0.197	0.485	25.822	0.424	72	69	63	78	124	102 original
1359	11 Succinic acid	15 Alanine	64	0.181	0.346	13.376	0.543	73	68	72	69	71	51 original
1408	11 Succinic acid	64 [799; Tyramine (3TMS)]	63	0.176	0.338	5.928	0.412	74	67	74	67	10	110 original
1484	11 Succinic acid	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49	0.121	0.183	16.674	0.390	75	66	78	63	83	120 original
1477	11 Succinic acid	133 [855; Squalene]	64	0.112	0.056	7.351	0.354	76	65	81	60	21	136 original
1453	11 Succinic acid	109 Octadecanoic acid	64	0.102	0.034	18.001	0.401	77	64	73	68	94	117 original
1391	11 Succinic acid	47 [NA]	64	0.100	0.075	10.784	0.421	78	63	80	61	50	105 original
1437	11 Succinic acid	93 [607; Putrescine (4TMS)]	60	0.098	0.204	18.222	0.385	79	62	77	64	97	123 original
1423	11 Succinic acid	79 Glucose	64	0.088	0.492	29.715	0.506	80	61	62	79	134	63 original
1434	11 Succinic acid	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	64	0.053	-0.038	5.981	0.389	81	60	84	57	11	121 original
1438	11 Succinic acid	94 Hexadecanoic acid	64	0.048	0.257	16.782	0.399	82	59	76	65	85	118 original
1482	11 Succinic acid	138 [674; Ergosterol (1TMS)]	46	-0.005	0.055	17.670	0.377	83	58	82	59	91	128 original
1462	11 Succinic acid	118 [928; Glucopyranose-6-phosphate (6TMS)]	58	-0.011	0.107	10.465	0.437	84	57	79	62	45	95 original
1485	11 Succinic acid	141 Lanosta-8,24-dien-3-beta-ol	61	-0.012	0.015	15.551	0.396	85		83	58	78	119 original

1483	11	Succinic acid	139	[700; Ergosta-5,7-dien-3-ol]	38	-0.013	-0.156	19,315	0.404	86	55	89	52	104	113 original
1397	11	Succinic acid	53	Glycerol-2-phosphate	64	-0.053	-0.155	12,876	0.359	87	54	88	53	65	135 original
1481	11	Succinic acid	137	Ergosterol	64	-0.056	-0.094	11,554	0.351	88	53	85	56	56	137 original
1415	11	Succinic acid	71	[731; Erythrose (3TMS)]	64	-0.058	-0.137	7,248	0.380	89	52	87	54	20	125 original
1451	11	Succinic acid	107	9-(Z)-Octadecenoic acid	64	-0.064	-0.240	9,978	0.368	90	51	92	49	42	130 original
1463	11	Succinic acid	119	[931; myo-Inositol-2-phosphate (7TMS)]	64	-0.108	-0.135	7,689	0.404	91	50	86	55	24	115 original
1416	11	Succinic acid	72	[919; D-Xylopyranose (4TMS)]	63	-0.130	-0.239	11,095	0.368	92	49	91	50	52	131 original
1480	11	Succinic acid	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.147	-0.238	4,265	0.444	93	48	90	51	6	93 original
1407	11	Succinic acid	63	Glutamine	52	-0.176	-0.652	18,436	0.621	94	47	121	20	100	10 original
1468	11	Succinic acid	124	[734; 1-Monooleoylglycerol (2TMS); 1-Monoheptadecanoylglycerol (1TMS)]	59	-0.185	-0.388	25,401	0.379	95	48	96	45	123	126 original
10367	11	Succinic acid	4	Phosphoric acid	51	-0.202	-0.380	29,548	0.323	96	45	95	46	133	138 duplicate
10772	11	Succinic acid	7	Threonine	64	-0.224	-0.394	25,337	0.404	97	44	98	43	121	114 duplicate
1396	11	Succinic acid	52	[NA]	46	-0.231	-0.621	21,797	0.586	98	43	114	27	115	29 original
1405	11	Succinic acid	61	[NA]	64	-0.249	-0.291	6,568	0.468	99	42	94	47	14	78 original
1442	11	Succinic acid	98	[997; Ribose-5-phosphate methoxymine (5TMS)]	48	-0.254	-0.663	20,598	0.515	100	41	122	19	110	60 original
1474	11	Succinic acid	130	Trehalose	63	-0.259	-0.390	24,955	0.377	101	40	97	44	120	127 original
1452	11	Succinic acid	108	Octadecenoic acid	64	-0.266	-0.438	9,601	0.387	102	39	101	40	38	122 original
1387	11	Succinic acid	43	[548; Leucine (2TBS)]	60	-0.270	-0.405	7,382	0.410	103	38	99	42	22	111 original
1402	11	Succinic acid	58	[636; 4R-Acetalamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	-0.300	-0.410	12,878	0.384	104	37	100	41	67	124 original
1419	11	Succinic acid	75	Lysine	48	-0.318	-0.500	35,075	0.403	105	36	103	38	137	116 original
1369	11	Succinic acid	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.328	-0.817	18,016	0.602	106	35	136	5	95	22 original
1410	11	Succinic acid	66	Glycine acid-3-phosphate	64	-0.338	-0.544	8,710	0.463	107	34	109	32	31	83 original
10092	11	Succinic acid	2	Serine	62	-0.341	-0.559	17,878	0.418	108	33	110	31	92	108 duplicate
1380	11	Succinic acid	36	[596; N-Acetylglutamic acid (2TMS)]	64	-0.343	-0.543	24,394	0.424	109	32	108	33	119	103 original
1404	11	Succinic acid	60	Glycerol-3-phosphate	64	-0.344	-0.483	16,895	0.420	110	31	102	39	86	106 original
1367	11	Succinic acid	23	Homoserine	64	-0.345	-0.787	12,396	0.574	111	30	132	9	63	34 original
1412	11	Succinic acid	68	[570; Hypoxanthine (2TMS)]	20	-0.347	-0.866	15,259	0.470	112	29	139	2	77	77 original
1381	11	Succinic acid	37	Phenylalanine	64	-0.357	-0.542	17,987	0.414	113	28	107	34	93	109 original
1411	11	Succinic acid	67	Citric acid	64	-0.372	-0.511	18,884	0.364	114	27	104	37	101	133 original
10905	11	Succinic acid	8	Isoleucine	55	-0.382	-0.534	17,318	0.373	115	26	105	36	88	129 duplicate
1371	11	Succinic acid	27	[815; (E)-4-Methyl-5-hydroxy-3-pentan-2-one (1TMS)]	53	-0.388	-0.798	21,298	0.540	116	25	134	7	113	53 original
1389	11	Succinic acid	45	Homocysteine	61	-0.391	-0.541	23,637	0.436	117	24	106	35	118	97 original
1433	11	Succinic acid	89	[775; Dopamine (4TMS)]	35	-0.392	-0.775	18,252	0.467	118	23	131	10	98	79 original
1375	11	Succinic acid	31	[622; Parabenic acid (2TMS)]	64	-0.404	-0.638	13,298	0.508	119	22	117	24	70	62 original
1439	11	Succinic acid	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	-0.417	-0.640	21,010	0.363	120	21	118	23	112	134 original
11037	11	Succinic acid	9	Proline	63	-0.420	-0.606	25,372	0.429	121	20	112	28	122	101 duplicate
1395	11	Succinic acid	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.425	-0.647	20,652	0.419	122	19	119	22	111	107 original
1378	11	Succinic acid	34	Aspartic acid	64	-0.446	-0.584	28,545	0.502	123	18	111	30	131	68 original
1393	11	Succinic acid	49	[877; Pyrophosphoric acid (4TMS)]	64	-0.450	-0.615	23,055	0.449	124	17	113	28	117	89 original
1399	11	Succinic acid	55	[612; 4-Aminobutyric acid (2TBS)]	63	-0.453	-0.694	22,746	0.461	125	16	124	17	116	85 original
1377	11	Succinic acid	33	Methionine	64	-0.461	-0.629	12,148	0.498	126	14	116	25	61	68 original
1392	11	Succinic acid	48	Asparagine	64	-0.461	-0.748	13,630	0.574	127	15	128	12	73	32 original
1376	11	Succinic acid	32	[728; N,N-Dimethyllysine methyl ester]	63	-0.485	-0.753	19,244	0.566	128	13	130	11	103	40 original
1374	11	Succinic acid	30	[815; Ethyl-3(2H)-thiophenone]	64	-0.495	-0.629	26,331	0.452	129	12	115	26	125	87 original
1475	11	Succinic acid	131	[626; 5-Methylthioadenosine (3TMS)]	55	-0.502	-0.652	18,333	0.442	130	11	120	21	99	94 original
10503	11	Succinic acid	5	Leucine	45	-0.511	-0.734	12,021	0.496	131	10	126	15	60	70 duplicate
10230	11	Succinic acid	3	Ethanolamine	62	-0.512	-0.745	14,075	0.483	132	9	128	13	74	72 duplicate
1364	11	Succinic acid	20	[619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.561	-0.813	15,855	0.549	133	8	135	6	79	48 original

1413	11	Succinic acid	69	Arginine	60	-0.562	-0.838	19,422	0.574	134	7	137	4	105	33	original
1421	11	Succinic acid	77	[826; beta-[[[5-methyl-2-phenyl]methyl]eneamino- benzenecarboxylic acid methyl ester]	62	-0.575	-0.742	26,995	0.464	135	6	127	14	129	81	original
1425	11	Succinic acid	81	Tyrosine	64	-0.577	-0.788	30,463	0.545	136	5	133	8	136	49	original
1403	11	Succinic acid	59	Ornithine; Arginine	64	-0.586	-0.669	36,449	0.471	137	4	123	18	139	78	original
1386	11	Succinic acid	42	Glutamic acid	60	-0.617	-0.733	27,616	0.475	138	3	125	16	130	73	original
1168	11	Succinic acid	80	Glycine	64	-0.620	-0.864	16,284	0.594	139	2	138	3	80	24	duplicate
1428	11	Succinic acid	82	Lysine	39	-0.641	-0.880	16,754	0.550	140	1	140	1	84	47	original
11299	12	Glycine acid	11	Succinic acid	63	0.752	0.892	11,874	0.585	1	140	9	132	49	25	duplicate
1487	12	Glycine acid	14	Fumaric acid	63	0.707	0.918	2,831	0.656	2	139	3	138	1	1	original
1502	12	Glycine acid	29	Erythritol	63	0.701	0.929	7,821	0.606	3	138	2	139	18	12	original
1497	12	Glycine acid	24	[725; 2-Ketooctanoic acid (2TMS)]	63	0.700	0.898	37,881	0.598	4	137	7	134	130	16	original
1489	12	Glycine acid	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	63	0.693	0.916	23,050	0.589	5	136	4	137	102	20	original
1511	12	Glycine acid	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	63	0.669	0.932	11,468	0.613	6	135	1	140	47	6	original
1501	12	Glycine acid	28	Malic acid	63	0.658	0.912	13,927	0.625	7	134	5	136	68	3	original
1527	12	Glycine acid	54	[NA]	55	0.647	0.826	6,533	0.540	8	133	21	120	10	47	original
1530	12	Glycine acid	57													
1512	12	Glycine acid	39	[757; 2-Desoxy-pentose-3-ylose dimethoxyamine (2TMS)]	55	0.634	0.807	15,811	0.623	9	132	25	116	76	4	original
1490	12	Glycine acid	62	[829; 1-Phenylethanol (1TMS)]	62	0.627	0.909	19,700	0.613	10	131	6	135	93	5	original
1486	12	Glycine acid	17	[700; 2-methyl-1,2-propanediol (2TMS)]	63	0.625	0.846	22,721	0.518	11	130	16	125	101	56	original
1538	12	Glycine acid	13	Uracil	63	0.624	0.887	20,967	0.589	12	129	10	131	96	21	original
1561	12	Glycine acid	65	[646; 3-Deoxyglucitol (5TMS)]	62	0.617	0.855	12,044	0.610	13	128	14	127	53	9	original
1529	12	Glycine acid	88	Gluconic acid	63	0.615	0.861	15,623	0.613	14	127	13	128	73	7	original
1519	12	Glycine acid	56	[829; Orotic acid (3TMS)]	63	0.611	0.841	9,272	0.611	15	126	19	122	31	8	original
1607	12	Glycine acid	46	Arabinose	63	0.607	0.823	20,717	0.595	16	125	22	119	95	17	original
1559	12	Glycine acid	134	Isomaltose	63	0.605	0.850	29,922	0.602	17	124	15	126	116	14	original
1602	12	Glycine acid	86	[793; D-Galactono-1,4-lactone (4TMS)]	60	0.601	0.784	25,147	0.582	18	123	28	113	107	26	original
1535	12	Glycine acid	129	[840; Maltose methoxyamine (6TMS); alpha-D-Glc-(1,4)-D- Glc]	58	0.596	0.844	11,915	0.588	19	122	17	124	50	23	original
1573	12	Glycine acid	62	[812; D-Xylofuranose (4TMS)]	63	0.592	0.779	19,493	0.570	20	121	29	112	91	31	original
1494	12	Glycine acid	100	[857; Mannitol (6TMS)]	63	0.586	0.832	13,283	0.561	21	120	20	121	61	35	original
1523	12	Glycine acid	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	63	0.585	0.817	22,025	0.572	22	119	23	118	97	29	original
1495	12	Glycine acid	50	[746; Ribonic acid-1,4-lactone (3TMS)]	60	0.577	0.841	8,730	0.589	23	118	18	123	23	19	original
1585	12	Glycine acid	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	51	0.576	0.897	4,018	0.608	24	117	8	133	2	11	original
1499	12	Glycine acid	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	62	0.570	0.793	6,839	0.497	25	116	27	114	12	62	original
1575	12	Glycine acid	26	Citramalic acid	63	0.557	0.807	22,145	0.554	26	115	24	117	99	39	original
1608	12	Glycine acid	102	[904; Galactose methoxyamine (5TMS)]	63	0.551	0.746	6,148	0.550	27	114	32	109	8	42	original
1513	12	Glycine acid	135													
1572	12	Glycine acid	63	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	63	0.544	0.720	17,708	0.487	28	113	38	103	87	65	original
1588	12	Glycine acid	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	63	0.528	0.802	40,732	0.552	29	112	26	115	133	41	original
1549	12	Glycine acid	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	40	0.510	0.891	5,476	0.577	30	111	12	129	4	28	original
1578	12	Glycine acid	115	Glucose-6-phosphate	61	0.504	0.691	30,317	0.557	31	110	43	98	118	38	original
1565	12	Glycine acid	76	Fructose	63	0.494	0.712	30,963	0.535	32	109	40	101	119	51	original
1589	12	Glycine acid	105	[705; 2-Ketogluconic acid (5TMS)]	48	0.493	0.773	13,851	0.536	33	108	30	111	66	50	original
1551	12	Glycine acid	92	[680; Glycerol-2-phosphate (4TMS)]	54	0.483	0.576	8,705	0.491	34	107	56	85	34	64	original
1593	12	Glycine acid	116	[882; Pseudouridine (5TMS)]	30	0.485	0.640	7,010	0.404	35	106	46	95	13	110	original
1508	12	Glycine acid	78	Mannose	61	0.478	0.689	8,840	0.497	36	105	44	97	25	61	original
1576	12	Glycine acid	120	[945; Uridine (3TMS)]	54	0.470	0.380	16,285	0.604	37	104	65	76	79	13	original
1598	12	Glycine acid	35	Pyroglutamic acid	63	0.470	0.698	47,529	0.510	38	103	42	99	138	58	original
	12	Glycine acid	103	[648; Ethylamine (2TMS)]	62	0.464	0.732	16,641	0.512	39	102	36	105	83	57	original
	12	Glycine acid	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	63	0.463	0.586	37,790	0.485	40	101	53	88	129	67	original



1579	12	Glyceric acid	106	733; Threitol (4TMS))	61	0.455	0.733	13.551	0.563	41	100	35	106	65	33 original
1605	12	Glyceric acid	132	[895; Isomaltose methoxyamine (8TMS))	42	0.454	0.885	10.081	0.610	42	89	11	130	37	10 original
1580	12	Glyceric acid	117	[724; Glycerol (3TMS))	55	0.441	0.741	8.287	0.553	43	98	34	107	20	40 original
1558	12	Glyceric acid	85	[528; Methylcitric acid (4TMS))	47	0.434	0.708	8.445	0.481	44	97	41	100	21	68 original
1563	12	Glyceric acid	110	[715; Erythritol (4TMS))	53	0.417	0.730	9.227	0.625	45	96	37	104	30	2 original
1491	12	Glyceric acid	18	[590; 1-Acetyl-2-thiohydantoin	63	0.415	0.620	12.067	0.457	46	95	49	92	54	77 original
1543	12	Glyceric acid	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS))	56	0.414	0.420	23.956	0.390	47	94	64	77	103	121 original
1594	12	Glyceric acid	121	[657; Erythritol (4TMS))	54	0.405	0.648	6.417	0.527	48	93	45	98	9	55 original
1570	12	Glyceric acid	97	[756; beta-D-Methylglucopyranoside (4TMS))	52	0.403	0.585	24.406	0.453	49	92	54	87	104	80 original
1601	12	Glyceric acid	128	[824; D-Sedoheptulose-7-phosphate (7TMS))	45	0.402	0.743	10.516	0.559	50	91	33	108	42	37 original
1546	12	Glyceric acid	73	[708; Glucose methoxyamine (5TMS))	56	0.397	0.630	9.453	0.424	51	90	48	93	32	36 original
1595	12	Glyceric acid	122	[844; Erythritol (4TMS))	52	0.395	0.765	9.124	0.560	52	89	31	110	28	88 original
1517	12	Glyceric acid	44	[910; 2-Ketogluconic acid methoxyamine (4TMS))	50	0.393	0.715	11.773	0.534	53	88	39	102	48	53 original
1547	12	Glyceric acid	74	[912; Tetradecanoic acid (1TMS))	63	0.391	0.614	10.119	0.472	54	87	50	91	38	69 original
9954	12	Glyceric acid	1	[938; Sulfuric acid (2TMS))	36	0.349	0.466	7.392	0.538	55	86	60	81	16	48 duplicate
1574	12	Glyceric acid	63	0.335	63	0.335	0.611	13.468	0.427	56	85	51	90	64	87 original
1584	12	Glyceric acid	91	[766; beta-D-Methylglucopyranoside (4TMS))	63	0.330	0.567	19.024	0.412	57	84	57	84	89	102 original
1599	12	Glyceric acid	126	[559; Erythritol (4TMS))	45	0.313	0.588	6.669	0.588	58	83	52	89	11	22 original
1586	12	Glyceric acid	113	Galactose-6-phosphate	61	0.296	0.560	7.499	0.405	59	81	58	83	17	107 original
1557	12	Glyceric acid	84	Mannitol	61	0.296	0.547	37.190	0.420	60	82	59	82	128	94 original
1600	12	Glyceric acid	127	[777; Fructose-6-phosphate methoxyamine (6TMS))	39	0.287	0.632	8.138	0.600	61	80	47	94	7	15 original
1597	12	Glyceric acid	114	Fructose-6-phosphate	52	0.287	0.579	5.579	0.456	62	79	55	86	8	78 original
1569	12	Glyceric acid	6	Glycerol	48	0.273	0.291	10.491	0.286	63	78	72	89	41	140 original
1584	12	Glyceric acid	111	[583; Erythritol (4TMS))	63	0.270	0.465	48.124	0.395	64	77	61	80	140	116 duplicate
1566	12	Glyceric acid	42	0.245	42	0.245	0.368	12.399	0.401	65	76	68	73	56	113 original
1560	12	Glyceric acid	59	[607; Putrescine (4TMS))	59	0.244	0.371	9.085	0.394	66	75	67	74	27	117 original
1492	12	Glyceric acid	87	[945; beta-D-Glucopyranose (5TMS))	61	0.242	0.446	41.288	0.420	67	74	63	78	138	86 original
1582	12	Glyceric acid	19	Alanine (BP) (3TMS)	63	0.208	0.450	17.057	0.441	68	73	62	79	85	81 original
1514	12	Glyceric acid	109	Octadecanoic acid	63	0.189	0.379	27.640	0.403	69	72	66	75	112	111 original
1566	12	Glyceric acid	48	0.186	48	0.186	0.266	7.335	0.423	70	71	74	67	15	91 original
1514	12	Glyceric acid	83	Sorbitol	57	0.178	-0.294	27.272	0.375	71	70	95	46	110	125 original
1587	12	Glyceric acid	41	[639; Proline (2TMS))	63	0.151	0.320	19.323	0.417	72	68	69	72	90	89 original
1563	12	Glyceric acid	94	Hexadecanoic acid	63	0.151	0.317	27.410	0.396	73	69	70	71	111	114 original
1577	12	Glyceric acid	90	[910; 9-(Z)-Hexadecenoic acid (1TMS))	63	0.138	0.112	11.945	0.344	74	67	78	63	51	136 original
1614	12	Glyceric acid	104	[795; Erythritol (4TMS))	62	0.137	0.286	10.963	0.384	75	66	73	68	44	123 original
1596	12	Glyceric acid	141	Lanosta-8,24-dien-3-beta-ol	60	0.130	0.197	7.039	0.432	76	65	77	64	14	84 original
1610	12	Glyceric acid	123	[945; Galactofuranose-6-phosphate (7TMS))	63	0.110	0.227	16.282	0.389	77	64	76	65	80	122 original
1553	12	Glyceric acid	137	Ergosterol	63	0.084	0.003	19.631	0.375	78	63	84	57	92	126 original
1606	12	Glyceric acid	133	[855; Squalene]	63	0.058	0.292	36.720	0.422	79	62	71	70	127	92 original
1488	12	Glyceric acid	15	Alanine	63	0.054	-0.024	12.126	0.354	80	61	85	56	55	134 original
1544	12	Glyceric acid	71	[731; Erythrose (3TMS))	63	0.035	0.055	24.574	0.548	81	60	82	59	105	44 original
1520	12	Glyceric acid	47	[NA]	63	0.033	-0.113	17.887	0.402	82	59	90	51	88	112 original
1611	12	Glyceric acid	138	[674; Ergosterol (1TMS))	45	0.030	0.068	9.026	0.430	84	57	80	61	26	88 original
1580	12	Glyceric acid	107	9-(Z)-Octadecenoic acid	63	0.030	-0.104	20.527	0.349	85	56	88	53	94	135 original
1592	12	Glyceric acid	119	[931; myo-Inositol-2-phosphate (7TMS))	63	0.029	0.077	12.489	0.424	86	55	79	62	57	90 original
1537	12	Glyceric acid	64	[789; Tyramine (3TMS))	62	0.027	0.065	8.284	0.360	87	54	81	60	19	132 original
1612	12	Glyceric acid	139	[700; Ergosta-5,7-dien-3-ol]	38	0.021	-0.091	11.009	0.341	88	53	87	54	45	137 original
1526	12	Glyceric acid	53	Glycerol-2-phosphate	63	0.012	-0.075	5.478	0.355	89	52	86	55	5	133 original
1552	12	Glyceric acid	79	Glucose	63	-0.055	0.250	41.280	0.460	90	51	75	66	135	73 original

1597	12	Glyceric acid	124	734; 1-Monoleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)	58	-0.072	-0.281	14,755	0.368	91	50	94	47	70	130	original
1525	12	Glyceric acid	52	[NA]	45	-0.095	-0.368	15,203	0.458	92	49	96	45	71	75	original
1536	12	Glyceric acid	63	Glutamine	51	-0.115	-0.521	16,079	0.545	93	48	107	34	78	46	original
1591	12	Glyceric acid	118	[928; Glucopyranose-6-phosphate (6TMS)]	57	-0.134	-0.106	9,489	0.411	94	47	89	52	33	103	original
1534	12	Glyceric acid	61	[NA]	57	-0.169	-0.230	10,461	0.390	95	46	91	50	40	119	original
1609	12	Glyceric acid	138	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.176	-0.232	4,607	0.409	96	45	92	49	3	104	original
1545	12	Glyceric acid	72	[919; D-Xylopyranose (4TMS)]	62	-0.187	-0.275	10,545	0.371	97	44	93	48	43	128	original
1581	12	Glyceric acid	108	Octadecenoic acid	63	-0.211	-0.422	9,161	0.405	98	43	98	43	29	108	original
10773	12	Glyceric acid	7	Threonine	63	-0.231	-0.467	36,646	0.381	99	42	101	40	125	124	duplicate
1533	12	Glyceric acid	60	Glycerol-3-phosphate	63	-0.236	-0.403	27,836	0.420	100	41	97	44	113	95	original
1528	12	Glyceric acid	55	[612; 4-Aminobutyric acid (2TBS)]	42	-0.243	-0.452	14,641	0.404	101	40	100	41	69	109	original
1568	12	Glyceric acid	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	49	-0.248	-0.488	12,493	0.372	102	39	105	38	58	127	original
1540	12	Glyceric acid	67	Citric acid	63	-0.251	-0.432	30,123	0.338	103	38	99	42	117	138	original
1510	12	Glyceric acid	37	Phenylalanine	63	-0.263	-0.524	29,156	0.422	104	37	108	33	115	93	original
1541	12	Glyceric acid	68	[570; Hypoxanthine (2TMS)]	19	-0.263	-0.835	10,298	0.419	105	36	138	3	39	97	original
1524	12	Glyceric acid	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	43	-0.269	-0.674	12,809	0.472	106	35	122	19	59	70	original
1498	12	Glyceric acid	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.293	-0.864	15,762	0.591	107	34	140	1	75	18	original
1493	12	Glyceric acid	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	30	-0.301	-0.605	11,112	0.548	108	33	116	25	46	43	original
1562	12	Glyceric acid	89	[775; Dopamine (4TMS)]	34	-0.301	-0.632	15,586	0.396	109	32	118	23	72	115	original
10368	12	Glyceric acid	4	Phosphoric acid	50	-0.309	-0.481	39,653	0.335	110	31	103	38	132	139	duplicate
15016	12	Glyceric acid	43	[548; Leucine (2TBS)]	59	-0.314	-0.475	13,246	0.392	111	30	102	39	60	118	original
10906	12	Glyceric acid	8	Isoleucine	54	-0.317	-0.556	24,951	0.360	112	29	110	31	106	131	duplicate
1603	12	Glyceric acid	130	Trehalose	62	-0.339	-0.481	36,228	0.408	113	28	104	37	122	105	original
10504	12	Glyceric acid	5	Leucine	44	-0.340	-0.772	11,961	0.532	114	27	132	9	52	54	duplicate
1521	12	Glyceric acid	48	Asparagine	63	-0.347	-0.652	16,394	0.547	115	26	120	21	81	45	original
1518	12	Glyceric acid	45	Homocysteine	60	-0.350	-0.538	13,453	0.416	116	25	109	32	63	100	original
1509	12	Glyceric acid	36	[596; N-Acetylglutamic acid (2TMS)]	63	-0.359	-0.575	35,286	0.417	117	24	113	28	121	98	original
1604	12	Glyceric acid	131	[626; 5-Methylthioadenosine (3TMS)]	54	-0.360	-0.569	9,921	0.430	118	23	112	29	35	85	original
1504	12	Glyceric acid	31	[622; Parabanic acid (2TMS)]	63	-0.365	-0.676	8,679	0.536	119	22	124	17	22	49	original
1571	12	Glyceric acid	98	[697; Ribose-5-phosphate methoxamine (5TMS)]	47	-0.367	-0.749	13,318	0.535	120	21	130	11	62	52	original
1522	12	Glyceric acid	49	[877; Pyrophosphoric acid (4TMS)]	63	-0.375	-0.561	15,758	0.441	121	20	111	30	74	83	original
1486	12	Glyceric acid	23	Homoserine	63	-0.391	-0.835	16,398	0.585	122	19	139	2	82	24	original
1539	12	Glyceric acid	66	Glyceric acid-3-phosphate	63	-0.403	-0.625	8,840	0.456	123	18	117	24	24	79	original
10231	12	Glyceric acid	3	Ethanolamine	61	-0.413	-0.655	9,959	0.424	124	17	121	20	36	89	duplicate
1507	12	Glyceric acid	34	Aspartic acid	63	-0.413	-0.601	39,463	0.486	125	16	114	27	131	66	original
1506	12	Glyceric acid	33	Methionine	63	-0.417	-0.676	16,067	0.499	126	15	123	18	77	60	original
1548	12	Glyceric acid	75	Lysine	63	-0.419	-0.605	46,304	0.390	127	14	115	26	137	120	original
1531	12	Glyceric acid	58	[636; 4R-Acetylido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	63	-0.425	-0.520	22,615	0.370	128	12	106	35	100	129	original
1503	12	Glyceric acid	30	[815; Ethyl-3(2H)-thiophenone]	63	-0.425	-0.678	36,692	0.415	129	13	126	15	126	101	original
1542	12	Glyceric acid	69	Arginine	59	-0.454	-0.828	28,125	0.566	130	11	136	5	114	32	original
11038	12	Glyceric acid	9	Proline	62	-0.457	-0.677	34,372	0.441	131	10	125	16	120	82	duplicate
1550	12	Glyceric acid	77	[826; beta-[(5-methyl-2-thenyl)methyl]eneamino-benzeneacetic acid methyl ester]	61	-0.461	-0.720	36,528	0.459	132	9	128	13	123	74	original
10093	12	Glyceric acid	2	Serine	61	-0.466	-0.634	25,330	0.407	133	8	119	22	108	106	duplicate
1500	12	Glyceric acid	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	52	-0.475	-0.832	17,099	0.563	134	7	137	4	86	34	original
1505	12	Glyceric acid	32	[729; N,N-Dimethyllysine methyl ester]	62	-0.480	-0.810	16,733	0.578	135	6	134	7	84	27	original
1554	12	Glyceric acid	81	Tyrosine	63	-0.494	-0.723	40,758	0.492	136	5	129	12	134	63	original
1515	12	Glyceric acid	42	Glutamic acid	59	-0.495	-0.770	36,567	0.472	137	4	131	10	124	71	original

11169	12	Glyceric acid	10	Glycine	63	-508	-0.818	25,728	0.570	138	3	135	6	109	30	duplicate
1532	12	Glyceric acid	59	Ornithine; Arginine	63	-522	-0.692	47,580	0.463	139	2	127	14	139	72	original
1555	12	Glyceric acid	82	Lysine	38	-528	-0.803	22,143	0.506	140	1	133	8	98	59	original
1617	13	Uracil	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	867	0.988	3,841	0.721	1	140	2	139	1	2	original
1658	13	Uracil	57	[757; 2-Desoxy-pentose-3-ylose dimethoxyamine (2TMS)]	55	867	0.959	10,545	0.662	2	139	11	130	27	21	original
1657	13	Uracil	56	[829; Orotic acid (3TMS)]	64	850	0.975	15,688	0.703	3	138	6	135	58	4	original
1625	13	Uracil	24	[725; 2-Ketooctanoic acid (2TMS)]	64	845	0.989	17,600	0.734	4	137	1	140	71	1	original
1735	13	Uracil	134	Isomaltose	64	843	0.983	9,580	0.710	5	136	3	138	17	3	original
1647	13	Uracil	46	Arabinose	64	840	0.968	7,877	0.695	6	135	8	133	8	10	original
1666	13	Uracil	65	[846; 3-Deoxyglucitol (5TMS)]	63	840	0.977	15,950	0.699	7	134	5	136	81	6	original
1730	13	Uracil	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	834	0.968	13,140	0.666	8	133	9	132	39	19	original
1640	13	Uracil	39	[828; 1-Phenylethanol (1TMS)]	63	804	0.979	5,338	0.688	9	132	4	137	3	12	original
1687	13	Uracil	86	[793; D-Galactono-1,4-lactone (4TMS)]	61	800	0.943	11,303	0.703	10	131	14	127	33	5	original
1651	13	Uracil	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	787	0.970	28,517	0.661	11	130	7	134	129	22	original
1618	13	Uracil	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	791	0.932	3,857	0.618	12	129	16	125	2	43	original
1655	13	Uracil	54	[NA]	55	760	0.924	20,010	0.578	13	128	18	123	90	65	original
1630	13	Uracil	29	Erythritol	64	753	0.959	14,004	0.657	14	127	12	129	41	23	original
1689	13	Uracil	88	Gluconic acid	64	749	0.928	6,947	0.691	15	126	17	124	6	11	original
11300	13	Uracil	11	Succinic acid	64	712	0.907	10,230	0.611	16	125	21	120	22	48	duplicate
1663	13	Uracil	62	[812; D-Xylofuranose (4TMS)]	64	701	0.898	5,897	0.636	17	124	22	119	4	33	original
1639	13	Uracil	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	691	0.961	9,975	0.676	18	123	10	131	20	14	original
1700	13	Uracil	99	[682; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	690	0.963	19,216	0.666	19	122	13	128	84	18	original
1615	13	Uracil	14	Fumaric acid	64	679	0.940	18,831	0.641	20	121	15	126	80	29	original
1693	13	Uracil	92	[680; Glycerol-2-phosphate (4TMS)]	54	676	0.760	14,628	0.561	21	120	41	100	51	72	original
1706	13	Uracil	105	[705; 2-Ketogluconic acid (5TMS)]	48	674	0.895	10,963	0.639	22	119	23	118	30	31	original
1704	13	Uracil	103	[648; Ethylamine (2TMS)]	63	665	0.864	10,632	0.604	23	118	26	115	28	53	original
1698	13	Uracil	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	638	0.819	10,493	0.562	24	117	31	110	26	71	original
11429	13	Uracil	12	Glyceric acid	63	624	0.887	20,967	0.589	25	116	25	116	98	58	duplicate
1623	13	Uracil	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	599	0.916	20,249	0.623	26	115	20	121	93	41	original
1629	13	Uracil	28	Malic acid	64	595	0.921	8,731	0.663	27	114	19	122	14	20	original
1671	13	Uracil	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	591	0.591	8,476	0.551	28	113	58	83	10	79	original
1677	13	Uracil	76	Fructose	64	581	0.858	11,182	0.667	29	112	27	114	32	17	original
1674	13	Uracil	73	[708; Glucose methoxyamine (5TMS)]	57	575	0.753	14,849	0.569	30	111	43	98	53	68	original
1707	13	Uracil	106	[733; Threitol (4TMS)]	62	574	0.851	10,200	0.698	31	110	28	113	21	9	original
1679	13	Uracil	78	Mannose	62	556	0.798	16,965	0.597	32	109	35	106	67	55	original
1702	13	Uracil	101	[832; Dopamine (4TMS)]	64	552	0.768	11,662	0.558	33	108	39	102	35	74	original
9955	13	Uracil	1	[938; Sulfuric acid (2TMS)]	36	549	0.686	16,330	0.605	34	107	50	91	63	52	duplicate
1692	13	Uracil	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	548	0.729	14,687	0.525	35	106	45	96	52	89	original
1641	13	Uracil	40	[690; 2,3-Dimethylsuccinic acid (2TMS)]	64	544	0.838	22,015	0.614	36	105	29	112	99	44	original
1627	13	Uracil	26	Citramalic acid	64	520	0.793	7,640	0.571	37	104	37	104	7	66	original
1622	13	Uracil	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	511	0.772	6,589	0.569	38	103	38	103	5	69	original
1726	13	Uracil	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	507	0.766	17,979	0.589	39	102	40	101	73	59	original
1698	13	Uracil	87	[945; beta-D-Glucopyranose (5TMS)]	62	497	0.720	21,828	0.508	40	101	47	94	98	99	original
1716	13	Uracil	115	Glucose-6-phosphate	62	487	0.813	11,157	0.629	41	100	34	107	31	37	original
1729	13	Uracil	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	487	0.816	10,908	0.581	42	99	33	108	29	63	original
1636	13	Uracil	35	Pyroglutamic acid	64	486	0.820	28,009	0.620	43	98	30	111	126	42	original
1721	13	Uracil	120	[945; Uridine (3TMS)]	54	438	0.364	8,702	0.644	44	97	71	70	13	27	original
1711	13	Uracil	110	[715; Erythritol (4TMS)]	54	428	0.795	18,310	0.671	45	96	36	105	75	16	original
10640	13	Uracil	6	Glycerol	64	428	0.677	28,825	0.553	46	95	51	90	132	76	duplicate

1718	13 Uracil	117	[724; Glyceral (3TMS)]	56	0.425	0.759	15.220	0.607	47	94	42	99	55	51 original
1722	13 Uracil	121	[657; Erythritol (4TMS)]	55	0.421	0.710	23.659	0.635	48	93	49	82	107	34 original
1686	13 Uracil	85	[529; Methylcitric acid (4TMS)]	48	0.406	0.711	9.174	0.515	49	92	48	83	15	98 original
1723	13 Uracil	122	[644; Erythritol (4TMS)]	52	0.403	0.818	24.220	0.624	50	91	32	109	110	40 original
1701	13 Uracil	100	[857; Mannitol (6TMS)]	64	0.372	0.730	9.759	0.558	51	90	44	97	18	75 original
1703	13 Uracil	102	[904; Galactose methoxamine (5TMS)]	64	0.358	0.638	16.417	0.544	52	89	56	85	64	82 original
1713	13 Uracil	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.353	0.662	27.475	0.546	53	88	54	87	124	80 original
1645	13 Uracil	44	[910; 2-Ketogluconic acid methoxamine (4TMS)]	50	0.340	0.724	12.630	0.631	54	87	46	95	37	36 original
1681	13 Uracil	80	[772; D-Glucose (5TMS)]	62	0.325	0.597	18.066	0.477	55	86	57	84	74	112 original
1733	13 Uracil	132	[895; Isomaltose methoxamine (6TMS)]	42	0.319	0.889	22.855	0.611	56	85	24	117	102	49 original
1620	13 Uracil	19	Alanine (BP) (3TMS)	64	0.313	0.583	8.532	0.544	57	84	59	82	11	81 original
1619	13 Uracil	18	[590; 1-Acetyl-2-thiohydantoin]	64	0.287	0.517	11.532	0.482	58	83	64	77	34	107 original
1736	13 Uracil	135		64	0.284	0.545	8.656	0.510	59	82	62	79	12	98 original
1728	13 Uracil	127	[777; Fructose-6-phosphate methoxamine (6TMS)]	39	0.277	0.677	14.238	0.614	60	81	52	89	46	45 original
1705	13 Uracil	104	[795; Erythritol (4TMS)]	63	0.269	0.444	14.033	0.553	61	80	66	75	43	77 original
1675	13 Uracil	74	[912; Tetradecanoic acid (1TMS)]	64	0.268	0.550	16.467	0.560	62	79	61	80	65	73 original
1714	13 Uracil	113	Galactose-6-phosphate	62	0.264	0.673	16.956	0.564	63	78	53	88	66	70 original
1717	13 Uracil	116	[882; Pseudouridine (5TMS)]	30	0.260	0.396	12.799	0.418	64	77	68	73	38	130 original
1642	13 Uracil	41	[638; Proline (2TMS)]	64	0.232	0.428	8.384	0.493	65	76	67	74	9	105 original
1648	13 Uracil	47	[NA]	64	0.215	0.253	16.162	0.477	66	75	75	66	82	111 original
1685	13 Uracil	84	Mannitol	62	0.211	0.555	19.142	0.495	67	74	60	81	83	102 original
1715	13 Uracil	114	Fructose-6-phosphate	53	0.209	0.652	17.907	0.604	68	73	55	86	72	54 original
1697	13 Uracil	98	myo-Inositol	49	0.202	0.213	27.842	0.318	69	72	78	63	125	140 original
1694	13 Uracil	93	[607; Putrescine (4TMS)]	60	0.199	0.366	26.202	0.435	70	71	70	71	116	125 original
1724	13 Uracil	123	[945; Galactofuranose-6-phosphate (7TMS)]	64	0.160	0.384	9.564	0.571	71	70	69	72	16	67 original
1727	13 Uracil	128	[559; Erythritol (4TMS)]	45	0.160	0.523	17.457	0.642	72	69	63	78	69	28 original
1616	13 Uracil	15	Alanine	64	0.117	0.260	10.423	0.655	73	68	73	68	25	25 original
1680	13 Uracil	79	Glucose	64	0.080	0.477	22.237	0.592	74	67	65	76	101	57 original
1654	13 Uracil	53	Glycerol-2-phosphate	64	0.074	0.004	22.095	0.401	75	66	83	58	100	133 original
1665	13 Uracil	64	[789; Tyramine (3TMS)]	63	0.069	0.193	15.765	0.439	76	65	79	62	59	122 original
1712	13 Uracil	111	[583; Erythritol (4TMS)]	42	0.066	0.257	30.268	0.434	77	64	74	67	136	128 original
1741	13 Uracil	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	49	0.063	0.230	24.466	0.494	78	63	76	65	111	104 original
1691	13 Uracil	90	[910; 9-(Z)-Hexadecanoic acid (1TMS)]	64	0.059	0.043	13.718	0.400	79	62	82	59	40	134 original
1684	13 Uracil	83	Sorbitol	58	0.053	-0.361	15.373	0.397	80	61	83	48	57	136 original
1734	13 Uracil	133	[855; Squalene]	64	0.035	-0.022	15.287	0.433	81	60	84	57	56	127 original
1710	13 Uracil	109	Octadecanoic acid	64	-0.003	0.313	14.127	0.522	82	59	72	69	44	90 original
1719	13 Uracil	118	[928; Glucopyranose-6-phosphate (6TMS)]	58	-0.020	0.156	18.544	0.431	83	58	80	61	77	128 original
1695	13 Uracil	94	Hexadecanoic acid	64	-0.038	0.222	12.526	0.538	84	57	77	64	36	85 original
1742	13 Uracil	141	Lanosta-8,24-dien-3-beta-ol	61	-0.059	0.076	24.010	0.519	85	56	81	60	109	92 original
1673	13 Uracil	72	[919; D-Xylopyranose (4TMS)]	63	-0.082	-0.146	19.306	0.368	86	55	87	54	86	137 original
1740	13 Uracil	139	[700; Ergosta-5,7-dien-3-ol]	38	-0.087	-0.148	27.091	0.450	87	54	88	53	123	120 original
1664	13 Uracil	63	Glutamine	52	-0.092	-0.688	26.567	0.698	88	53	114	27	117	7 original
1708	13 Uracil	107	9-(Z)-Octadecenoic acid	64	-0.114	-0.224	10.404	0.400	89	52	90	51	24	135 original
1739	13 Uracil	138	[674; Ergosterol (1TMS)]	46	-0.129	-0.026	26.122	0.515	90	51	85	56	115	95 original
1720	13 Uracil	119	[931; myo-Inositol-2-phosphate (7TMS)]	64	-0.150	-0.110	14.997	0.532	91	50	86	55	54	86 original
1738	13 Uracil	137	Ergosterol	64	-0.150	-0.170	14.267	0.480	92	49	89	52	48	109 original
10369	13 Uracil	4	Phosphoric acid	51	-0.172	-0.480	24.734	0.337	93	48	98	43	112	139 duplicate
1644	13 Uracil	43	[548; Leucine (2TBS)]	60	-0.181	-0.409	14.343	0.479	94	47	95	46	50	110 original
1725	13 Uracil	124	[734; 1-Monodecylglycerol (2TMS); 1-Monohexadecylglycerol (1TMS)]	59	-0.219	-0.334	34.565	0.442	95	46	92	49	140	121 original

1626	13 Uracil	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.232	-0.900	26,718	0.628	96	45	135	6	118	38 original
1731	13 Uracil	130	Trehalose	63	-0.246	-0.362	18,979	0.403	97	44	94	47	81	132 original
1653	13 Uracil	52	[NA]	46	-0.256	-0.577	29,838	0.672	98	43	102	39	135	15 original
1672	13 Uracil	71	[731; Erythrose (3TMS)]	64	-0.270	-0.517	10,327	0.489	99	42	91	50	23	108 original
1659	13 Uracil	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	-0.286	-0.498	14,232	0.425	100	41	100	41	45	129 original
1737	13 Uracil	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.309	-0.449	9,938	0.439	101	40	96	45	19	123 original
1709	13 Uracil	108	Oxalacetic acid	64	-0.327	-0.490	19,057	0.407	102	39	99	42	82	131 original
1676	13 Uracil	75	Lysine	64	-0.340	-0.601	28,869	0.468	103	38	103	38	134	114 original
1662	13 Uracil	61	[NA]	64	-0.342	-0.458	15,902	0.472	104	37	97	44	60	113 original
1699	13 Uracil	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	48	-0.355	-0.796	28,733	0.592	105	38	122	19	130	56 original
1624	13 Uracil	23	Homoserine	64	-0.401	-0.865	20,022	0.613	106	35	131	10	91	48 original
10774	13 Uracil	7	Threonine	64	-0.403	-0.603	19,779	0.453	107	34	104	37	89	118 duplicate
1628	13 Uracil	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	-0.403	-0.863	28,922	0.580	108	33	129	12	131	64 original
1637	13 Uracil	36	[596; N-Acetylglutamic acid (2TMS)]	64	-0.409	-0.644	20,123	0.463	109	32	108	33	92	116 original
1648	13 Uracil	45	Homocysteine	61	-0.424	-0.617	32,871	0.437	110	31	106	35	139	124 original
1699	13 Uracil	88	[570; Hypoxanthine (2TMS)]	20	-0.432	-0.924	19,616	0.610	111	30	137	4	87	50 original
1650	13 Uracil	49	[877; Pyrophosphoric acid (4TMS)]	64	-0.437	-0.569	32,239	0.494	112	29	101	40	138	103 original
10094	13 Uracil	2	Serine	62	-0.454	-0.681	20,736	0.481	113	28	113	28	95	108 duplicate
1621	13 Uracil	31	[619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxethylamine (4TMS)]	31	-0.471	-0.892	19,262	0.656	114	27	133	8	85	24 original
1732	13 Uracil	55	[626; 5-Methylthioadenosine (3TMS)]	55	-0.481	-0.652	26,971	0.626	115	26	109	32	121	39 original
1690	13 Uracil	89	[775; Dopamine (4TMS)]	35	-0.482	-0.799	23,608	0.585	116	25	123	18	105	60 original
1667	13 Uracil	68	Glycine acid-3-phosphate	64	-0.501	-0.715	18,573	0.519	117	23	115	28	79	81 original
1632	13 Uracil	31	[622; Parabenic acid (2TMS)]	64	-0.501	-0.758	23,188	0.517	118	24	120	21	103	94 original
10907	13 Uracil	8	Isoleucine	55	-0.508	-0.611	18,568	0.383	119	22	105	38	78	138 duplicate
1661	13 Uracil	60	Glycerol-3-phosphate	64	-0.517	-0.652	14,031	0.529	120	21	110	31	42	87 original
1696	13 Uracil	95	[770; 3,4,6-Tris(hydroxyphenyl)ethanolamine (5TMS)]	50	-0.527	-0.642	28,856	0.553	121	20	107	34	133	78 original
1635	13 Uracil	34	Aspartic acid	64	-0.540	-0.677	23,793	0.500	122	19	111	30	108	101 original
1638	13 Uracil	37	Phenylalanine	64	-0.556	-0.755	14,238	0.513	123	18	118	23	47	97 original
1039	13 Uracil	9	Proline	63	-0.557	-0.722	24,934	0.453	124	17	116	25	113	117 duplicate
1649	13 Uracil	48	Asparagine	64	-0.563	-0.827	21,282	0.639	125	16	125	16	97	32 original
1634	13 Uracil	33	Methionine	64	-0.570	-0.744	19,761	0.519	126	15	117	24	88	93 original
1668	13 Uracil	67	Citric acid	64	-0.572	-0.678	14,323	0.452	127	14	112	28	49	119 original
1652	13 Uracil	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.609	-0.855	27,022	0.540	128	13	127	14	122	83 original
1631	13 Uracil	30	[815; Ethyl-3(2H)-thiophenone]	64	-0.632	-0.757	23,429	0.465	129	12	119	22	104	115 original
1633	13 Uracil	32	[729; N,N-Dimethyllysine methyl ester]	63	-0.643	-0.895	28,494	0.634	130	11	134	7	128	35 original
10505	13 Uracil	5	Leucine	45	-0.667	-0.879	17,541	0.582	131	10	132	9	70	62 duplicate
1660	13 Uracil	59	Ornithine; Arginine	64	-0.668	-0.773	30,407	0.507	132	9	121	20	137	100 original
1656	13 Uracil	55	[612; 4-Aminobutyric acid (2TBS)]	43	-0.674	-0.801	28,273	0.582	133	8	124	17	127	61 original
1670	13 Uracil	69	Arginine	60	-0.690	-0.937	20,308	0.640	134	7	138	3	94	30 original
10232	13 Uracil	3	Ethanolamine	62	-0.702	-0.848	23,650	0.613	135	6	126	15	108	47 duplicate
1643	13 Uracil	42	Glutamic acid	60	-0.727	-0.860	26,927	0.527	136	5	128	13	119	88 original
11770	13 Uracil	10	Glycine	64	-0.737	-0.957	17,100	0.698	137	4	139	2	68	8 duplicate
1678	13 Uracil	77	[826; beta-[(5-methyl-2-thienyl)methyleneamino-benzeneacetic acid methyl ester]	62	-0.740	-0.863	25,289	0.539	138	3	130	11	114	84 original
1683	13 Uracil	82	Lysine	39	-0.779	-0.971	18,486	0.654	139	2	140	1	76	26 original
1682	13 Uracil	81	Tyrosine	64	-0.802	-0.918	26,934	0.683	140	1	136	5	120	13 original
1756	14 Fumaric acid	28	Malic acid	64	0.825	0.978	11,647	0.681	1	140	1	140	57	1 original
11301	14 Fumaric acid	11	Succinic acid	64	0.782	0.926	9,627	0.633	2	139	8	133	37	13 duplicate
11430	14 Fumaric acid	12	Glycic acid	63	0.707	0.918	2,831	0.656	3	138	12	129	1	4 duplicate

1752	14 Fumaric acid	24	[725; 2-Ketoclanonic acid (2TMS)]	64	0.700	0.936	35.615	0.633	4	137	5	138	130	14 original
1768	14 Fumaric acid	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.689	0.950	9.261	0.644	5	136	2	139	36	10 original
1744	14 Fumaric acid	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	0.688	0.935	20.929	0.641	6	135	6	135	101	11 original
11558	14 Fumaric acid	13	Uracil	64	0.679	0.940	18.831	0.641	7	134	3	138	95	12 duplicate
1754	14 Fumaric acid	26	Citramalic acid	64	0.677	0.874	19.951	0.595	8	133	23	118	98	34 original
1790	14 Fumaric acid	62	[812; D-Xylofuranose (4TMS)]	64	0.676	0.885	17.259	0.610	9	132	19	122	89	30 original
1750	14 Fumaric acid	22	[690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.674	0.925	5.199	0.614	10	131	10	131	6	28 original
1757	14 Fumaric acid	29	Erythritol	64	0.670	0.930	5.559	0.655	11	130	7	134	8	5 original
1814	14 Fumaric acid	86	[793; D-Galactono-1,4-lactone (4TMS)]	61	0.668	0.882	23.376	0.630	12	129	20	121	107	15 original
1749	14 Fumaric acid	21	[678; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	64	0.654	0.856	19.909	0.602	13	128	28	113	97	33 original
1767	14 Fumaric acid	39	[829; 1-Phenylethanol (1TMS)]	63	0.653	0.939	17.925	0.667	14	127	4	137	93	3 original
1768	14 Fumaric acid	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.649	0.875	38.730	0.617	15	126	22	119	133	23 original
1843	14 Fumaric acid	115	Glucose-6-phosphate	62	0.644	0.809	28.120	0.575	16	125	35	106	118	44 original
1784	14 Fumaric acid	58	[829; Orolic acid (3TMS)]	64	0.640	0.908	8.395	0.650	17	124	16	125	27	6 original
1778	14 Fumaric acid	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	0.637	0.916	10.811	0.606	18	123	13	128	48	31 original
1785	14 Fumaric acid	57	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55	0.634	0.902	14.285	0.646	19	122	17	124	70	7 original
1804	14 Fumaric acid	76	Fructose	64	0.633	0.830	28.738	0.566	20	121	31	110	119	48 original
1793	14 Fumaric acid	65	[646; 3-Deoxyglucitol (5TMS)]	63	0.631	0.922	11.359	0.668	21	120	11	130	53	2 original
1862	14 Fumaric acid	134	Isomaltose	64	0.631	0.925	27.848	0.645	22	119	9	132	116	8 original
1774	14 Fumaric acid	46	Arabinose	64	0.628	0.900	18.923	0.645	23	118	18	123	98	9 original
1834	14 Fumaric acid	106	[733; Threitol (4TMS)]	62	0.622	0.858	11.540	0.622	24	117	26	115	56	18 original
1782	14 Fumaric acid	54	[NA]	55	0.616	0.857	7.100	0.579	25	116	27	114	18	42 original
1806	14 Fumaric acid	78	Mannose	62	0.613	0.817	7.694	0.525	26	115	33	108	21	65 original
1857	14 Fumaric acid	129	[840; Maltose methoxyamine (6TMS); alpha-D-Glc-(1,4)-D-Glc]	59	0.610	0.910	10.681	0.583	27	114	15	126	45	40 original
1763	14 Fumaric acid	35	Pyroglutamic acid	64	0.607	0.813	45.490	0.564	28	113	34	107	138	51 original
1816	14 Fumaric acid	88	Gluconic acid	64	0.606	0.878	13.684	0.613	29	112	21	120	64	28 original
1745	14 Fumaric acid	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	0.598	0.863	20.616	0.566	30	111	25	116	100	49 original
1860	14 Fumaric acid	132	[895; Isomaltose methoxyamine (8TMS)]	42	0.570	0.911	10.990	0.585	31	110	14	127	50	38 original
1853	14 Fumaric acid	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	0.563	0.722	35.554	0.547	32	109	45	96	129	58 original
1849	14 Fumaric acid	121	[657; Erythritol (4TMS)]	55	0.562	0.779	7.525	0.580	33	108	39	102	19	41 original
1845	14 Fumaric acid	117	[724; Glycerol (3TMS)]	56	0.561	0.822	6.890	0.578	34	107	32	109	14	43 original
1828	14 Fumaric acid	100	[857; Mannitol (6TMS)]	64	0.559	0.791	11.196	0.529	35	106	36	105	52	61 original
1798	14 Fumaric acid	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	0.554	0.555	21.808	0.428	36	105	61	80	103	106 original
1830	14 Fumaric acid	102	[904; Galactose methoxyamine (5TMS)]	64	0.551	0.728	4.165	0.528	37	104	44	97	3	64 original
1838	14 Fumaric acid	110	[715; Erythritol (4TMS)]	54	0.540	0.832	8.887	0.627	38	103	30	111	33	17 original
1840	14 Fumaric acid	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.536	0.781	8.836	0.504	39	102	38	103	31	71 original
1850	14 Fumaric acid	122	[644; Erythritol (4TMS)]	52	0.534	0.852	10.079	0.564	40	101	29	112	42	50 original
1801	14 Fumaric acid	73	[708; Glucose methoxyamine (5TMS)]	57	0.521	0.736	8.107	0.458	41	100	43	98	23	87 original
1848	14 Fumaric acid	120	[945; Uridine (3TMS)]	54	0.516	0.347	14.457	0.616	42	99	73	68	71	25 original
1820	14 Fumaric acid	92	[680; Glycerol-2-phosphate (4TMS)]	54	0.500	0.653	8.250	0.478	43	98	54	87	26	79 original
1813	14 Fumaric acid	85	[529; Methylictric acid (4TMS)]	48	0.498	0.783	6.231	0.498	44	97	37	104	12	74 original
1802	14 Fumaric acid	74	[912; Tetradecanoic acid (1TMS)]	64	0.484	0.706	8.622	0.485	45	95	48	93	28	76 original
1863	14 Fumaric acid	135	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	0.484	0.702	15.545	0.469	46	96	49	92	79	82 original
1831	14 Fumaric acid	103	[648; Ethylamine (2TMS)]	63	0.476	0.747	15.171	0.539	47	94	40	101	75	59 original
1772	14 Fumaric acid	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	0.468	0.747	10.345	0.559	48	93	41	100	44	53 original
1746	14 Fumaric acid	18	[590; 1-Acetyl-2-thiohydantoin]	64	0.463	0.657	9.900	0.466	49	92	53	88	39	83 original
1854	14 Fumaric acid	126	[559; Erythritol (4TMS)]	45	0.463	0.682	5.906	0.570	50	91	50	91	9	46 original
1842	14 Fumaric acid	114	Fructose-6-phosphate	53	0.460	0.720	4.612	0.510	51	90	48	95	4	68 original

1844	14 Fumaric acid	116 [882; Pseudouridine (5TMS)]	30 0,457	0,502	6,949	0,404	52	89	63	78	15	119 original
1841	14 Fumaric acid	113 Galactose-6-phosphate	62 0,433	0,679	5,944	0,442	53	88	51	90	10	98 original
1856	14 Fumaric acid	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45 0,432	0,743	9,025	0,519	54	87	42	99	34	89 original
1747	14 Fumaric acid	19 Alanine (BP) (3TMS)	64 0,430	0,661	14,596	0,462	55	86	52	89	73	84 original
10641	14 Fumaric acid	6 Glycerol	64 0,386	0,597	46,091	0,441	56	85	59	82	140	99 duplicate
1855	14 Fumaric acid	127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	39 0,358	0,639	5,024	0,570	57	84	55	88	5	47 original
1833	14 Fumaric acid	105 [705; 2-Ketogluconic acid (5TMS)]	48 0,356	0,710	12,735	0,559	58	83	47	94	63	52 original
1827	14 Fumaric acid	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41 0,354	0,865	6,288	0,591	59	82	24	117	13	35 original
1829	14 Fumaric acid	101 [832; Dopamine (4TMS)]	64 0,353	0,613	11,849	0,474	60	81	58	83	58	81 original
1769	14 Fumaric acid	41 [839; Proline (2TMS)]	64 0,347	0,534	16,908	0,459	61	80	62	79	88	86 original
1815	14 Fumaric acid	87 [945; beta-D-Glucopyranose (5TMS)]	62 0,345	0,614	38,962	0,445	62	79	57	84	134	95 original
1819	14 Fumaric acid	91 [766; beta-D-Methylglucopyranoside (4TMS)]	64 0,339	0,565	17,880	0,443	63	78	60	81	92	96 original
1825	14 Fumaric acid	97 [756; beta-D-Methylglucopyranoside (4TMS)]	52 0,336	0,627	22,774	0,440	64	77	56	85	105	101 original
1839	14 Fumaric acid	111 [583; Erythritol (4TMS)]	42 0,331	0,452	14,136	0,424	65	76	67	74	67	109 original
1832	14 Fumaric acid	104 [795; Erythritol (4TMS)]	63 0,319	0,475	8,662	0,439	66	75	66	75	29	102 original
1824	14 Fumaric acid	96 myo-Inositol	49 0,313	0,286	12,356	0,307	67	74	75	66	60	140 original
1851	14 Fumaric acid	123 [945; Galactofuranose-6-phosphate (7TMS)]	64 0,293	0,447	13,870	0,450	68	73	68	73	66	91 original
1811	14 Fumaric acid	83 Sorbitol	58 0,251	-0,220	25,260	0,391	69	72	94	47	110	125 original
1837	14 Fumaric acid	109 Octadecanoic acid	64 0,221	0,487	25,555	0,410	70	71	64	77	112	116 original
1868	14 Fumaric acid	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49 0,219	0,336	8,878	0,441	71	70	74	67	32	100 original
1861	14 Fumaric acid	133 [855; Squalene]	64 0,207	0,133	9,934	0,378	72	69	81	60	40	130 original
1808	14 Fumaric acid	80 [772; D-Glucose (5TMS)]	62 0,203	0,481	34,385	0,415	73	68	65	76	123	114 original
1743	14 Fumaric acid	15 Alanine	64 0,177	0,237	22,209	0,584	74	67	76	65	104	39 original
1822	14 Fumaric acid	94 Hexadecanoic acid	64 0,173	0,419	25,284	0,407	75	66	71	70	111	118 original
1792	14 Fumaric acid	64 [789; Tyramine (3TMS)]	63 0,167	0,214	6,160	0,371	76	65	79	62	11	134 original
1812	14 Fumaric acid	84 Mannitol	62 0,150	0,435	35,483	0,445	77	64	69	72	128	93 original
1866	14 Fumaric acid	138 [674; Ergosterol (1TMS)]	46 0,142	0,206	10,248	0,383	78	63	80	81	43	128 original
1864	14 Fumaric acid	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17 0,132	0,046	3,651	0,417	79	62	85	56	2	113 original
1807	14 Fumaric acid	79 Glucose	64 0,132	0,432	39,064	0,506	80	61	70	71	135	70 original
9956	14 Fumaric acid	1 [938; Sulfuric acid (2TMS)]	36 0,127	0,367	7,238	0,523	81	60	72	69	18	67 duplicate
1859	14 Fumaric acid	141 Lanosta-8,24-dien-3-beta-ol	61 0,127	0,226	7,800	0,412	82	59	77	64	22	115 original
1818	14 Fumaric acid	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	64 0,072	0,079	9,977	0,370	83	58	83	58	41	135 original
1865	14 Fumaric acid	137 Ergosterol	64 0,063	0,008	17,808	0,398	84	57	87	54	91	120 original
1821	14 Fumaric acid	93 [607; Putrescine (4TMS)]	60 0,042	0,220	10,738	0,377	85	56	78	63	46	131 original
1867	14 Fumaric acid	139 [700; Ergosta-5,7-dien-3-ol]	38 0,041	-0,026	12,461	0,364	86	55	88	53	62	136 original
1775	14 Fumaric acid	47 [NA]	64 0,029	0,062	12,426	0,430	87	54	84	57	61	105 original
1846	14 Fumaric acid	118 [928; Glucopyranose-6-phosphate (6TMS)]	58 0,022	0,117	8,153	0,375	88	53	82	59	24	132 original
1835	14 Fumaric acid	107 9-(Z)-Octadecenoic acid	64 -0,007	-0,103	18,447	0,384	89	52	90	51	94	127 original
1847	14 Fumaric acid	119 [931; myo-Inositol-2-phosphate (7TMS)]	64 -0,019	0,020	10,803	0,408	90	51	88	55	47	117 original
1799	14 Fumaric acid	71 [731; Erythrose (3TMS)]	64 -0,020	-0,105	15,745	0,424	91	50	91	50	80	110 original
1781	14 Fumaric acid	53 Glycerol-2-phosphate	64 -0,027	-0,094	5,476	0,350	92	49	89	52	7	138 original
1852	14 Fumaric acid	124 [734; 1-Monodoleoylglycerol (2TMS); 1-Monohexadecenoylethanol (1TMS)]	59 -0,044	-0,196	16,570	0,362	93	48	92	49	86	137 original
10370	14 Fumaric acid	4 Phosphoric acid	51 -0,151	-0,374	37,743	0,379	94	47	96	45	132	128 duplicate
1800	14 Fumaric acid	72 [919; D-Xylopyranose (4TMS)]	63 -0,152	-0,204	9,161	0,333	95	46	93	48	35	139 original
1858	14 Fumaric acid	130 Trehalose	63 -0,173	-0,315	34,245	0,374	96	45	95	46	122	133 original
10775	14 Fumaric acid	7 Threonine	64 -0,200	-0,435	34,660	0,422	97	44	100	41	124	112 duplicate
1766	14 Fumaric acid	58 [636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64 -0,232	-0,415	20,458	0,392	98	43	99	42	99	124 original
1836	14 Fumaric acid	108 Octadecanoic acid	64 -0,242	-0,397	7,659	0,395	99	42	98	43	20	122 original
1803	14 Fumaric acid	75 Lysine	64 -0,245	-0,495	44,364	0,443	100	41	103	38	137	97 original

1764	14 Fumaric acid	36	[596; N-Acetylglutamic acid (2TMS)]	64	-0.258	-0.507	33.324	0.425	101	40	105	36	121	108 original
1788	14 Fumaric acid	60	Glycerol-3-phosphate	64	-0.281	-0.439	25.833	0.445	102	39	101	40	113	94 original
1789	14 Fumaric acid	61	[NA]	64	-0.307	-0.378	8.786	0.423	103	38	97	44	30	111 original
1785	14 Fumaric acid	67	Citric acid	64	-0.313	-0.469	28.111	0.397	104	37	102	39	117	121 original
1780	14 Fumaric acid	52	[NA]	46	-0.320	-0.557	16.263	0.552	105	36	107	34	82	55 original
1765	14 Fumaric acid	37	Phenylalanine	64	-0.321	-0.561	27.145	0.449	106	35	108	33	115	92 original
1784	14 Fumaric acid	66	Glyceric acid-3-phosphate	64	-0.322	-0.588	7.146	0.477	107	34	110	31	17	80 original
1771	14 Fumaric acid	43	[548; Leucine (2TBS)]	60	-0.327	-0.508	11.398	0.425	108	33	106	35	55	107 original
1791	14 Fumaric acid	63	Glutamine	52	-0.332	-0.870	16.492	0.613	109	32	116	25	85	27 original
10095	14 Fumaric acid	2	Serine	62	-0.337	-0.578	23.508	0.435	110	31	109	32	108	104 duplicate
1826	14 Fumaric acid	98	[697; Ribose-5-phosphate methoxymine (5TMS)]	48	-0.362	-0.792	14.202	0.574	111	30	131	10	69	45 original
10908	14 Fumaric acid	8	Isoleucine	55	-0.390	-0.505	23.178	0.394	112	29	104	37	106	123 duplicate
1759	14 Fumaric acid	31	[622; Parabanic acid (2TMS)]	64	-0.392	-0.697	8.249	0.548	113	28	122	19	25	57 original
1751	14 Fumaric acid	23	Homoserine	64	-0.395	-0.872	14.937	0.628	114	27	134	7	74	16 original
1751	14 Fumaric acid	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	-0.409	-0.874	17.354	0.622	115	26	135	6	90	19 original
11040	14 Fumaric acid	9	Proline	63	-0.416	-0.625	32.574	0.437	116	25	111	30	120	103 duplicate
1753	14 Fumaric acid	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.422	-0.894	15.453	0.612	117	24	137	4	77	29 original
1748	14 Fumaric acid	20	[619; 2,3,4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.424	-0.767	11.951	0.821	118	23	127	14	59	21 original
1823	14 Fumaric acid	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	-0.468	-0.642	13.796	0.385	119	22	114	27	65	126 original
1773	14 Fumaric acid	45	Homocysteine	61	-0.477	-0.640	15.200	0.458	120	21	113	28	76	88 original
1761	14 Fumaric acid	33	Methionine	64	-0.483	-0.688	14.563	0.529	121	20	119	22	72	62 original
1782	14 Fumaric acid	34	Aspartic acid	64	-0.490	-0.646	37.610	0.533	122	19	115	26	131	60 original
1777	14 Fumaric acid	49	[877; Pyrophosphoric acid (4TMS)]	64	-0.492	-0.631	16.639	0.451	123	18	112	29	87	80 original
1780	14 Fumaric acid	32	[729; N,N-Dimethyllysine methyl ester]	63	-0.493	-0.800	16.309	0.821	124	17	132	9	83	20 original
10233	14 Fumaric acid	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.499	-0.749	14.165	0.549	125	16	125	16	68	56 original
1758	14 Fumaric acid	3	Ethanolamine	62	-0.508	-0.734	9.758	0.483	126	15	123	18	38	78 duplicate
1758	14 Fumaric acid	30	[815; Ethyl-3(2H)-thiophenone]	64	-0.511	-0.681	34.845	0.453	127	14	118	23	125	89 original
1783	14 Fumaric acid	55	[612; 4-Aminobutyric acid (2TBS)]	43	-0.513	-0.676	16.323	0.461	128	13	117	24	84	85 original
1817	14 Fumaric acid	89	[775; Dopamine (4TMS)]	35	-0.516	-0.774	16.169	0.524	129	12	128	13	81	66 original
1776	14 Fumaric acid	48	Asparagine	64	-0.517	-0.787	15.476	0.589	130	11	130	11	78	37 original
1859	14 Fumaric acid	131	[626; 5-Methylthioadenosine (3TMS)]	55	-0.537	-0.694	11.110	0.484	131	10	121	20	51	77 original
1787	14 Fumaric acid	59	Ornithine; Arginine	64	-0.537	-0.691	45.725	0.496	132	9	120	21	139	75 original
1786	14 Fumaric acid	68	[570; Hypoxanthine (2TMS)]	20	-0.537	-0.932	10.958	0.529	133	8	140	1	49	63 original
1805	14 Fumaric acid	77	[826; beta-[[[5-methyl-2-thienyl]methyl]amino]benzeneacetic acid methyl ester]	62	-0.540	-0.735	34.877	0.504	134	7	124	17	128	72 original
1797	14 Fumaric acid	69	Arginine	60	-0.546	-0.875	26.463	0.616	135	6	136	5	114	24 original
1809	14 Fumaric acid	81	Tyrosine	64	-0.550	-0.778	39.110	0.554	136	5	129	12	136	54 original
1770	14 Fumaric acid	42	Glutamic acid	60	-0.569	-0.755	34.891	0.503	137	4	126	15	127	73 original
10506	14 Fumaric acid	5	Leucine	45	-0.592	-0.846	11.382	0.589	138	3	133	8	54	36 duplicate
11171	14 Fumaric acid	10	Glycine	64	-0.626	-0.908	24.027	0.820	139	2	138	3	109	22 duplicate
1810	14 Fumaric acid	82	Lysine	39	-0.655	-0.909	21.303	0.606	140	1	139	2	102	32 original
1918	15 Alanine	64	[789; Tyramine (3TMS)]	63	-0.656	0.802	17.023	0.480	1	140	2	139	59	93 original
1933	15 Alanine	79	Glucose	64	-0.622	0.867	17.846	0.584	2	139	1	140	69	38 original
1977	15 Alanine	123	[945; Galactofuranose-6-phosphate (7TMS)]	64	-0.533	0.780	9.054	0.572	3	138	3	138	10	43 original
1968	15 Alanine	114	Fructose-6-phosphate	53	-0.507	0.752	18.175	0.537	4	137	5	136	72	69 original
1987	15 Alanine	113	Galactose-6-phosphate	62	-0.450	0.740	19.073	0.542	5	136	6	135	78	63 original
1873	15 Alanine	19	Alanine (BP) (3TMS)	64	-0.398	0.644	9.285	0.509	6	135	9	132	11	78 original
1958	15 Alanine	104	[795; Erythritol (4TMS)]	63	-0.354	0.493	16.040	0.541	7	134	16	125	50	65 original
1912	15 Alanine	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	-0.353	0.322	9.002	0.409	8	133	31	110	9	123 original



10642	15 Alanine	6	Glycerol	0.701	25,505	0.545	9	132	7	134	117	60 duplicate
1895	15 Alanine	64	41 [639; Proline (2TMS)]	0.491	7,980	0.455	10	131	18	123	5	105 original
1929	15 Alanine	64	75 Lysine	0.238	24,025	0.418	11	130	40	101	106	119 original
1889	15 Alanine	64	35 Pyroglutamic acid	0.663	25,005	0.599	12	129	8	133	113	29 original
1979	15 Alanine	64	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	0.755	15,386	0.594	13	128	4	137	48	32 original
1950	15 Alanine	49	96 myo-Inositol	0.171	29,968	0.344	14	127	54	87	130	139 original
1927	15 Alanine	57	73 [708; Glucose methoxamine (5TMS)]	0.492	19,811	0.542	15	126	17	124	86	64 original
1934	15 Alanine	62	80 [772; D-Glucose (5TMS)]	0.623	15,196	0.489	16	125	11	130	43	81 original
10086	15 Alanine	62	2 Serine	0.111	15,221	0.458	17	124	67	74	44	104 duplicate
1969	15 Alanine	62	115 Glucose-6-phosphate	0.269	9,385	0.611	18	123	10	131	13	24 original
1924	15 Alanine	57	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	0.563	6,819	0.508	19	122	14	127	1	80 original
1972	15 Alanine	58	118 [928; Glucopyranose-6-phosphate (6TMS)]	0.467	19,429	0.423	20	121	20	121	84	115 original
1932	15 Alanine	62	78 Mannose	0.480	20,844	0.531	21	120	19	122	97	71 original
1937	15 Alanine	58	83 Sorbitol	0.112	10,774	0.385	22	119	66	75	21	130 original
1882	15 Alanine	64	28 Malic acid	0.226	11,845	0.590	23	118	42	99	23	34 original
1930	15 Alanine	64	76 Fructose	0.611	11,212	0.612	24	117	12	129	22	23 original
1879	15 Alanine	48	25 [709; 2,5-Diaminovalerolactam (2TMS)]	0.426	23,815	0.586	25	116	25	116	105	36 original
1941	15 Alanine	62	87 [945; beta-D-Glucopyranose (5TMS)]	0.193	19,452	0.516	26	115	13	128	85	75 original
10776	15 Alanine	64	7 Threonine	0.192	15,175	0.414	27	114	60	81	42	120 duplicate
1970	15 Alanine	30	116 [882; Pseudouridine (5TMS)]	0.191	-0.270	0.420	28	113	11	30	51	118 original
1916	15 Alanine	64	62 [812; D-Xylofuranose (4TMS)]	0.184	7,520	0.605	29	112	21	120	3	27 original
1960	15 Alanine	62	106 [733; Threitol (4TMS)]	0.418	14,799	0.629	30	111	26	115	41	19 original
11302	15 Alanine	64	11 Succinic acid	0.181	13,376	0.543	31	110	29	112	27	62 duplicate
11686	15 Alanine	64	14 Fumaric acid	0.177	22,209	0.584	32	108	41	100	101	37 duplicate
1880	15 Alanine	64	26 Citramalic acid	0.177	7,185	0.517	33	109	47	94	2	73 original
10371	15 Alanine	51	4 Phosphoric acid	0.172	10,801	0.357	34	107	68	73	83	136 duplicate
1990	15 Alanine	17	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	0.162	8,629	0.391	35	106	34	107	7	127 original
1910	15 Alanine	64	56 [829; Orotic acid (3TMS)]	0.158	21,130	0.671	36	105	24	117	99	6 original
1945	15 Alanine	64	91 [766; beta-D-Methylglucopyranoside (4TMS)]	0.157	20,580	0.486	37	104	51	90	96	87 original
1920	15 Alanine	64	66 GlycERIC acid-3-phosphate	0.154	19,025	0.450	38	103	55	86	78	108 original
1870	15 Alanine	64	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	0.153	8,423	0.655	39	102	38	105	6	12 original
1872	15 Alanine	64	18 [590; 1-Acetyl-2-thiohydantoin]	0.152	13,664	0.412	40	101	37	104	29	121 original
1940	15 Alanine	61	86 [793; D-Galactono-1,4-lactone (4TMS)]	0.151	16,796	0.670	41	100	15	126	56	7 original
1956	15 Alanine	64	102 [904; Galactose methoxamine (5TMS)]	0.150	19,198	0.477	42	99	58	83	79	96 original
1984	15 Alanine	63	130 Trehalose	0.148	14,793	0.377	43	98	61	80	40	132 original
1875	15 Alanine	64	21 [878; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	0.148	7,750	0.509	44	97	50	91	4	79 original
1892	15 Alanine	64	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	0.146	14,191	0.595	45	96	45	96	30	30 original
1881	15 Alanine	53	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	0.145	28,928	0.567	46	95	86	55	128	46 original
1878	15 Alanine	64	24 [725; 2-Ketocacetic acid (2TMS)]	0.141	17,127	0.677	47	93	33	108	60	5 original
1894	15 Alanine	64	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	0.141	19,030	0.556	48	94	38	103	77	53 original
1865	15 Alanine	42	111 [583; Erythritol (4TMS)]	0.141	31,040	0.344	49	92	39	102	134	138 original
11041	15 Alanine	63	9 Proline	0.139	18,103	0.441	50	91	73	68	71	109 duplicate
1871	15 Alanine	64	17 [700; 2-methyl-1,2-propanediol (2TMS)]	0.138	8,890	0.568	51	90	30	111	8	45 original
1942	15 Alanine	64	88 Gluconic acid	0.134	13,473	0.638	52	89	32	109	28	17 original
1885	15 Alanine	64	31 [622; Parabenic acid (2TMS)]	0.132	23,598	0.492	53	88	72	69	104	83 original
1866	15 Alanine	63	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	0.126	30,021	0.482	54	87	59	82	132	89 original
1988	15 Alanine	64	134 Isomaltose	0.121	14,294	0.682	55	86	27	114	31	2 original
1883	15 Alanine	64	29 Erythritol	0.118	17,213	0.581	56	85	49	92	61	39 original
11559	15 Alanine	64	13 Urecl	0.117	10,423	0.655	57	84	35	106	19	13 duplicate
1987	15 Alanine	64	133 [855; Squalene]	0.112	16,301	0.349	58	83	64	77	53	137 original
1886	15 Alanine	63	32 [729; N,N-Dimethyllysine methyl ester]	0.104	26,395	0.586	59	82	80	61	121	35 original

1955	15 Alanine	101	[832; Dopamine (4TMS)]	64	0.103	0.176	17,005	0.533	60	81	52	89	58	70 original
1900	15 Alanine	46	Arabinose	64	0.102	0.445	15,263	0.682	61	80	23	118	47	3 original
1919	15 Alanine	65	[646; 3-Deoxyglucitol (5TMS)]	63	0.094	0.373	22,249	0.690	62	79	28	113	102	1 original
1986	15 Alanine	132	[895; Isomaltose methoxyamine (8TMS)]	42	0.092	-0.084	25,815	0.517	63	78	97	44	119	74 original
10909	15 Alanine	8	Isoleucine	55	0.091	0.019	14,457	0.387	64	77	83	58	32	129 duplicate
1893	15 Alanine	39	[829; 1-Phenylethanol (1TMS)]	63	0.091	0.214	14,542	0.624	65	76	46	95	34	20 original
1957	15 Alanine	103	[848; Ethylamine (2TMS)]	63	0.087	0.174	17,747	0.554	66	75	53	88	37	56 original
1897	15 Alanine	43	[548; Leucine (2TBS)]	60	0.085	0.156	14,557	0.491	67	74	57	84	35	88 original
1954	15 Alanine	100	[857; Mannitol (6TMS)]	64	0.082	0.036	12,827	0.496	68	73	77	64	26	82 original
1952	15 Alanine	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	48	0.082	-0.013	29,835	0.540	69	72	88	53	129	68 original
1887	15 Alanine	33	Methionine	64	0.080	0.009	17,463	0.474	70	71	85	56	85	97 original
1877	15 Alanine	23	Homoserine	64	0.073	-0.018	17,329	0.571	71	70	90	51	63	44 original
1874	15 Alanine	120	[845; Uridine (3TMS)]	54	0.071	0.015	9,911	0.566	72	69	84	57	16	47 original
135														
1989	15 Alanine	30	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	0.069	-0.016	9,353	0.469	73	68	89	52	12	98 original
1884	15 Alanine	85	[815; Ethyl-3(2H)-thiophenone]	64	0.064	0.036	17,000	0.466	74	67	78	63	57	100 original
1939	15 Alanine	138	[674; Ergosterol (1TMS)]	46	0.064	0.103	15,242	0.437	75	66	69	72	46	111 original
1992	15 Alanine	138	[674; Ergosterol (1TMS)]	46	0.053	0.117	25,418	0.388	76	65	65	76	116	128 original
1975	15 Alanine	121	[657; Erythritol (4TMS)]	55	0.048	0.166	26,569	0.541	77	64	56	85	123	68 original
1890	15 Alanine	36	[596; N-Acetylglutamic acid (2TMS)]	64	0.048	0.049	14,698	0.424	78	63	75	66	38	113 original
111431	15 Alanine	12	Glyceric acid	63	0.044	0.055	24,574	0.548	79	62	74	67	109	59 duplicate
1888	15 Alanine	34	Aspartic acid	64	0.042	0.023	18,415	0.461	80	61	81	60	73	102 original
1971	15 Alanine	117	[724; Glycerol (3TMS)]	56	0.017	0.087	19,216	0.513	81	60	71	70	82	76 original
1928	15 Alanine	74	[912; Tetradecanoic acid (1TMS)]	64	0.014	0.092	20,465	0.431	82	59	70	71	95	112 original
1891	15 Alanine	37	Phenylalanine	64	0.008	-0.109	9,802	0.481	83	58	98	43	15	91 original
1876	15 Alanine	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	-0.008	0.028	25,130	0.580	84	57	79	62	114	40 original
1904	15 Alanine	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	-0.015	0.135	32,347	0.555	85	56	62	79	136	54 original
1935	15 Alanine	81	Tyrosine	64	-0.016	-0.354	21,656	0.662	86	55	119	22	100	11 original
1925	15 Alanine	71	[731; Erythrose (3TMS)]	64	-0.018	-0.050	9,660	0.402	87	54	92	49	14	125 original
1983	15 Alanine	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	-0.020	0.217	19,715	0.664	88	53	44	97	87	10 original
1913	15 Alanine	59	Ornithine; Arginine	64	-0.021	-0.035	25,711	0.461	89	51	91	50	118	101 original
11172	15 Alanine	10	Glycine	64	-0.021	-0.332	12,422	0.667	90	52	117	24	25	8 duplicate
1901	15 Alanine	47	[NA]	64	-0.025	0.020	18,771	0.409	91	50	82	59	75	122 original
1923	15 Alanine	69	Arginine	60	-0.035	-0.173	14,505	0.603	92	49	101	40	33	28 original
1926	15 Alanine	72	[919; D-Xylopyranose (4TMS)]	63	-0.036	-0.081	20,973	0.336	93	48	95	48	98	140 original
1896	15 Alanine	42	Glutamic acid	60	-0.050	-0.083	20,077	0.492	94	47	96	45	90	84 original
1908	15 Alanine	54	[NA]	55	-0.052	0.193	24,418	0.559	95	46	48	93	107	52 original
1899	15 Alanine	45	Homocysteine	61	-0.056	-0.133	34,939	0.422	96	45	100	41	139	116 original
1953	15 Alanine	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	-0.061	-0.009	19,987	0.540	97	44	87	54	89	67 original
1814	15 Alanine	60	Glycerol-3-phosphate	64	-0.063	-0.247	10,033	0.478	98	43	107	34	17	95 original
1893	15 Alanine	139	[700; Ergosta-5,7-dien-3-ol]	38	-0.067	-0.264	26,551	0.371	99	42	110	31	122	133 original
		77	[826; beta-[[[5-methyl-2-thenyl)methyl]eneamino-benzeneacetic acid methyl ester]											
1931	15 Alanine	109	Octadecanoic acid	62	-0.085	-0.189	19,209	0.484	100	41	103	38	81	88 original
1863	15 Alanine	64	-0.102	0.047	14,667	0.451	101	40	76	65	37	107	original	
1994	15 Alanine	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	49	-0.105	-0.250	26,313	0.421	102	39	108	33	120	117 original
1905	15 Alanine	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.106	-0.232	31,026	0.551	103	38	106	35	133	57 original
1864	15 Alanine	110	[715; Erythritol (4TMS)]	54	-0.113	0.120	22,886	0.647	104	37	63	78	103	14 original
10234	15 Alanine	3	Ethanolamine	62	-0.117	-0.440	24,431	0.594	105	36	123	18	108	31 duplicate
10507	15 Alanine	5	Leucine	45	-0.117	-0.120	19,903	0.544	106	35	99	42	88	61 duplicate

57	15 Alanine	1911	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55	-0.126	0.223	17,517	0.680	107	34	43	98	66	4 original
	15 Alanine	1902	Asparagine	64	-0.128	-0.465	20,278	0.635	108	33	125	16	93	18 original
	15 Alanine	1915	[NA]	64	-0.152	-0.446	17,220	0.491	109	32	124	17	62	85 original
	15 Alanine	1946	[680; Glycerol-2-phosphate (4TMS)]	54	-0.154	0.445	17,919	0.564	110	31	22	119	70	49 original
	15 Alanine	9957	[938; Sulfuric acid (2TMS)]	36	-0.178	-0.224	15,871	0.512	111	30	105	36	49	77 duplicate
	15 Alanine	1985	[626; 5-Methylthioadenosine (3TMS)]	55	-0.180	-0.390	28,187	0.565	112	29	122	19	127	48 original
	15 Alanine	1948	Hexadecanoic acid	64	-0.181	-0.059	11,900	0.481	113	28	94	47	24	103 original
	15 Alanine	1962	Octadecanoic acid	64	-0.190	-0.296	20,303	0.382	114	27	113	28	94	131 original
	15 Alanine	1921	Citric acid	64	-0.197	-0.321	10,535	0.440	115	26	115	26	20	110 original
	15 Alanine	1978	[644; Erythritol (4TMS)]	52	-0.198	-0.218	28,896	0.551	116	25	104	37	125	58 original
	15 Alanine	1951	[756; beta-D-Methylglucopyranoside (4TMS)]	52	-0.205	-0.052	16,634	0.563	117	24	93	48	55	50 original
	15 Alanine	1981	[777; Fructose-6-phosphate methoxyamine (6TMS)]	39	-0.212	-0.564	15,226	0.563	118	23	129	12	45	51 original
	15 Alanine	1903	[877; Pyrophosphoric acid (4TMS)]	64	-0.212	-0.360	33,491	0.423	119	22	121	20	137	114 original
	15 Alanine	1907	Glycerol-2-phosphate	64	-0.227	-0.327	24,598	0.369	120	21	116	25	110	134 original
	15 Alanine	1978	[734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	59	-0.234	-0.355	36,053	0.361	121	20	120	21	140	135 original
	15 Alanine	1991	Ergosterol	64	-0.250	-0.281	14,568	0.454	122	19	112	29	36	108 original
	15 Alanine	1938	Mannitol	62	-0.265	-0.253	20,162	0.468	123	18	109	32	91	99 original
	15 Alanine	1980	[559; Erythritol (4TMS)]	45	-0.275	-0.490	20,231	0.613	124	17	127	14	92	21 original
	15 Alanine	1898	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	-0.277	-0.188	17,457	0.591	125	16	102	39	64	33 original
	15 Alanine	1922	[570; Hypoxanthine (2TMS)]	20	-0.284	-0.876	19,203	0.555	126	15	137	4	80	55 original
	15 Alanine	1995	Lanosta-8,24-dien-3-beta-ol	61	-0.302	-0.487	27,700	0.480	127	14	126	15	124	92 original
	15 Alanine	1909	[612; 4-Aminobutyric acid (2TBS)]	43	-0.307	-0.827	34,170	0.613	128	13	135	6	138	22 original
	15 Alanine	1947	[607; Putrescine (4TMS)]	60	-0.325	-0.339	30,019	0.479	129	12	118	23	131	94 original
	15 Alanine	1982	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	-0.341	-0.318	14,713	0.580	130	11	114	27	39	41 original
	15 Alanine	1936	Lysine	39	-0.366	-0.610	16,560	0.667	131	10	132	9	54	9 original
	15 Alanine	1944	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	64	-0.390	-0.556	16,278	0.406	132	9	128	13	52	124 original
	15 Alanine	1949	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	-0.401	-0.583	31,871	0.526	133	8	131	10	135	72 original
	15 Alanine	1874	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.415	-0.805	24,683	0.640	134	7	134	7	111	16 original
	15 Alanine	1961	9-(Z)-Octadecenoic acid	64	-0.422	-0.569	10,275	0.402	135	6	130	11	18	126 original
	15 Alanine	1973	[931; myo-Inositol-2-phosphate (7TMS)]	64	-0.501	-0.735	17,805	0.482	136	5	133	8	68	90 original
	15 Alanine	1906	[NA]	46	-0.507	-0.878	28,721	0.605	137	4	138	3	128	26 original
	15 Alanine	1943	[775; Dopamine (4TMS)]	35	-0.516	-0.898	24,699	0.577	138	3	139	2	112	42 original
	15 Alanine	1959	[705; 2-Ketogluconic acid (5TMS)]	48	-0.571	-0.828	18,522	0.642	139	2	136	5	74	15 original
	15 Alanine	1917	Glutamine	52	-0.609	-0.925	25,366	0.607	140	1	140	1	115	25 original
	16 [644; 2-Methyl-1,3-butanediol]	2003	[725; 2-Ketooctanoic acid (2TMS)]	64	0.942	0.984	14,933	0.734	1	140	1	140	49	1 original
	16 [644; 2-Methyl-1,3-butanediol]	2036	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55	0.868	0.944	13,530	0.662	2	139	14	127	39	24 original
	16 [644; 2-Methyl-1,3-butanediol]	1560	Uracil	64	0.867	0.988	3,841	0.721	3	138	2	139	2	3 duplicate
	16 [644; 2-Methyl-1,3-butanediol]	2025	Arabinose	64	0.862	0.963	11,148	0.705	4	137	9	132	27	6 original
	16 [644; 2-Methyl-1,3-butanediol]	2044	[646; 3-Deoxyglucitol (5TMS)]	63	0.861	0.974	19,310	0.699	5	136	6	135	81	8 original
	16 [644; 2-Methyl-1,3-butanediol]	2008	Erythritol	64	0.846	0.982	15,701	0.693	6	135	3	138	55	11 original
	16 [644; 2-Methyl-1,3-butanediol]	2035	[829; Orotic acid (3TMS)]	64	0.844	0.970	18,779	0.703	7	134	8	133	78	7 original
	16 [644; 2-Methyl-1,3-butanediol]	1996	[700; 2-methyl-1,2-propanediol (2TMS)]	64	0.840	0.948	2,832	0.645	8	133	13	128	1	31 original
	16 [644; 2-Methyl-1,3-butanediol]	2113	Isomaltose	64	0.829	0.973	9,602	0.710	9	132	7	134	16	5 original
	16 [644; 2-Methyl-1,3-butanediol]	2108	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	0.825	0.981	16,298	0.658	10	131	10	131	59	25 original
	16 [644; 2-Methyl-1,3-butanediol]	2018	[829; 1-Phenylethanol (1TMS)]	63	0.823	0.980	8,659	0.688	11	130	4	137	12	15 original
	16 [644; 2-Methyl-1,3-butanediol]	2065	[793; D-Galectono-1,4-lactone (4TMS)]	61	0.820	0.935	13,684	0.725	12	129	15	128	42	2 original

11303	16 [644; 2-Methyl-1,3-butar	11	Succinic acid	64	0.800	0.934	11,615	0.630	13	128	18	123	29	39 duplicate
2033	16 [644; 2-Methyl-1,3-butar	54	[NA]	55	0.790	0.934	22,037	0.596	14	127	17	124	102	56 original
2029	16 [644; 2-Methyl-1,3-butar	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	0.785	0.959	30,944	0.689	15	126	11	130	136	14 original
2017	16 [644; 2-Methyl-1,3-butar	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.783	0.978	11,754	0.693	16	125	5	136	30	10 original
2067	16 [644; 2-Methyl-1,3-butar	88	Gluconic acid	64	0.753	0.921	9,704	0.691	17	124	21	120	18	13 original
2041	16 [644; 2-Methyl-1,3-butar	62	[812; D-Xylofuranose (4TMS)]	64	0.733	0.897	4,992	0.662	18	123	23	118	4	23 original
11432	16 [644; 2-Methyl-1,3-butar	12	Glycetic acid	63	0.693	0.916	23,050	0.589	19	122	22	119	105	61 duplicate
2078	16 [644; 2-Methyl-1,3-butar	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	0.690	0.955	20,615	0.666	20	121	12	129	95	20 original
11687	16 [644; 2-Methyl-1,3-butar	14	Fumaric acid	64	0.688	0.935	20,929	0.641	21	120	16	125	97	32 duplicate
2007	16 [644; 2-Methyl-1,3-butar	103	[648; Ethylamine (2TMS)]	63	0.653	0.853	13,543	0.605	22	119	26	115	40	50 original
2062	16 [644; 2-Methyl-1,3-butar	28	Malic acid	64	0.647	0.927	9,735	0.663	23	118	19	122	19	22 original
2071	16 [644; 2-Methyl-1,3-butar	92	[680; Glycerol-2-phosphate (4TMS)]	54	0.642	0.745	16,449	0.561	24	117	44	97	61	72 original
2001	16 [644; 2-Methyl-1,3-butar	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.638	0.923	22,636	0.622	25	116	20	121	104	45 original
2084	16 [644; 2-Methyl-1,3-butar	105	[705; 2-Ketogluconic acid (5TMS)]	48	0.619	0.879	12,789	0.629	26	115	24	117	37	40 original
2052	16 [644; 2-Methyl-1,3-butar	73	[708; Glucose methoxyamine (5TMS)]	57	0.617	0.768	17,451	0.555	27	114	40	101	70	77 original
2055	16 [644; 2-Methyl-1,3-butar	76	Fructose	64	0.611	0.852	9,669	0.667	28	113	27	114	17	19 original
2049	16 [644; 2-Methyl-1,3-butar	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	0.602	0.581	6,453	0.497	29	112	58	83	6	103 original
2057	16 [644; 2-Methyl-1,3-butar	78	Mannose	62	0.589	0.795	19,538	0.597	30	111	34	107	85	54 original
2019	16 [644; 2-Methyl-1,3-butar	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.585	0.845	18,700	0.614	31	110	28	113	77	47 original
2076	16 [644; 2-Methyl-1,3-butar	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	0.581	0.793	11,900	0.576	32	109	38	105	31	66 original
2104	16 [644; 2-Methyl-1,3-butar	125	[692; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	0.568	0.764	15,699	0.589	33	108	41	100	54	62 original
2000	16 [644; 2-Methyl-1,3-butar	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	0.559	0.795	4,180	0.562	34	107	35	106	3	70 original
2080	16 [644; 2-Methyl-1,3-butar	101	[832; Dopamine (4TMS)]	64	0.550	0.757	14,033	0.562	35	106	42	99	43	71 original
2084	16 [644; 2-Methyl-1,3-butar	115	Glucose-6-phosphate	62	0.548	0.816	8,425	0.640	36	105	32	109	10	33 original
2014	16 [644; 2-Methyl-1,3-butar	35	Pyroglutamic acid	64	0.548	0.824	25,014	0.635	37	104	31	110	113	37 original
2085	16 [644; 2-Methyl-1,3-butar	106	[733; Threitol (4TMS)]	62	0.543	0.838	12,765	0.713	38	103	29	112	36	4 original
2005	16 [644; 2-Methyl-1,3-butar	26	Citramalic acid	64	0.542	0.793	5,267	0.547	39	102	37	104	5	80 original
9958	16 [644; 2-Methyl-1,3-butar	1	[938; Sulfuric acid (2TMS)]	36	0.533	0.660	17,033	0.588	40	101	55	86	67	63 duplicate
2070	16 [644; 2-Methyl-1,3-butar	91	[768; beta-D-Methylglucopyranoside (4TMS)]	64	0.508	0.716	17,143	0.522	41	100	46	95	68	92 original
2089	16 [644; 2-Methyl-1,3-butar	120	[945; Uridine (3TMS)]	54	0.477	0.412	8,442	0.648	42	99	68	73	11	30 original
2107	16 [644; 2-Methyl-1,3-butar	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.461	0.931	12,101	0.600	43	98	30	111	32	53 original
2079	16 [644; 2-Methyl-1,3-butar	100	[857; Mannitol (6TMS)]	64	0.457	0.777	10,642	0.558	44	97	39	102	23	73 original
2081	16 [644; 2-Methyl-1,3-butar	102	[904; Galactose methoxyamine (5TMS)]	64	0.439	0.697	18,040	0.546	45	96	50	91	73	81 original
10643	16 [644; 2-Methyl-1,3-butar	6	Glycerol	64	0.436	0.665	25,764	0.553	46	95	54	87	116	78 duplicate
2066	16 [644; 2-Methyl-1,3-butar	87	[945; beta-D-Glucopyranose (5TMS)]	62	0.435	0.676	19,713	0.508	47	94	52	89	88	99 original
2096	16 [644; 2-Methyl-1,3-butar	117	[724; Glycerol (3TMS)]	56	0.434	0.755	17,289	0.596	48	93	43	98	69	55 original
2091	16 [644; 2-Methyl-1,3-butar	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.434	0.701	29,506	0.544	49	92	49	92	129	83 original
2089	16 [644; 2-Methyl-1,3-butar	110	[715; Erythritol (4TMS)]	54	0.426	0.780	20,444	0.671	50	91	38	103	93	18 original
2100	16 [644; 2-Methyl-1,3-butar	121	[657; Erythritol (4TMS)]	55	0.424	0.705	25,555	0.640	51	90	48	93	115	34 original
2101	16 [644; 2-Methyl-1,3-butar	122	[644; Erythritol (4TMS)]	52	0.413	0.809	26,196	0.606	52	89	33	108	118	49 original
2064	16 [644; 2-Methyl-1,3-butar	85	[529; Methylcitric acid (4TMS)]	48	0.385	0.705	11,281	0.506	53	88	47	94	28	100 original
2111	16 [644; 2-Methyl-1,3-butar	132	[895; Isomaltose methoxyamine (8TMS)]	42	0.366	0.878	24,689	0.612	54	87	25	116	112	48 original
2114	16 [644; 2-Methyl-1,3-butar	135												
2114	16 [644; 2-Methyl-1,3-butar	135												
1997	16 [644; 2-Methyl-1,3-butar	18	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	0.365	0.590	7,863	0.511	55	86	57	84	7	97 original
2023	16 [644; 2-Methyl-1,3-butar	44	[590; 1-Acetyl-2-thiohydantoin]	64	0.350	0.549	12,504	0.465	56	85	60	81	34	117 original
2082	16 [644; 2-Methyl-1,3-butar	113	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	0.345	0.729	14,050	0.623	57	84	45	96	44	43 original
1988	16 [644; 2-Methyl-1,3-butar	127	Galactose-6-phosphate	62	0.338	0.696	19,007	0.586	58	83	51	90	80	64 original
2106	16 [644; 2-Methyl-1,3-butar	129	Alanine (BP) (3TMS)	64	0.275	0.547	9,282	0.544	59	82	61	80	14	82 original
2059	16 [644; 2-Methyl-1,3-butar	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.266	0.673	14,994	0.636	60	81	53	88	50	36 original
2093	16 [644; 2-Methyl-1,3-butar	80	[772; D-Glucose (5TMS)]	62	0.260	0.547	16,007	0.477	61	80	62	79	56	113 original
	16 [644; 2-Methyl-1,3-butar	114	Fructose-6-phosphate	53	0.257	0.652	19,659	0.604	62	79	56	85	87	51 original

2053	16 [644; 2-Methyl-1,3-butar 74	[912; Tetradecanoic acid (1TMS)]	64	0.252	0.546	18.491	0.555	63	78	63	78	75	76	original
2095	16 [644; 2-Methyl-1,3-butar 116	[882; Pseudouridine (5TMS)]	30	0.241	0.420	14.380	0.426	64	77	67	74	46	130	original
2093	16 [644; 2-Methyl-1,3-butar 104	[795; Erythritol (4TMS)]	63	0.241	0.422	15.637	0.576	65	76	66	75	52	65	original
2075	16 [644; 2-Methyl-1,3-butar 96	myo-Inositol	49	0.231	0.219	29.928	0.320	66	75	76	65	131	140	original
2063	16 [644; 2-Methyl-1,3-butar 84	Mannitol	62	0.222	0.568	16.683	0.494	67	74	59	82	65	105	original
2105	16 [644; 2-Methyl-1,3-butar 41	[559; Erythritol (4TMS)]	45	0.208	0.514	18.565	0.666	68	73	64	77	76	21	original
2020	16 [644; 2-Methyl-1,3-butar 41	[639; Proline (2TMS)]	64	0.192	0.379	7.880	0.504	69	72	69	72	8	102	original
2072	16 [644; 2-Methyl-1,3-butar 93	[607; Putrescine (4TMS)]	60	0.180	0.360	28.283	0.416	70	71	71	70	124	133	original
2028	16 [644; 2-Methyl-1,3-butar 47	[NA]	64	0.186	0.210	17.584	0.477	71	70	77	64	72	112	original
2102	16 [644; 2-Methyl-1,3-butar 83	[945; Galactofuranose-6-phosphate (7TMS)]	64	0.174	0.361	9.747	0.564	72	69	70	71	20	69	original
2062	16 [644; 2-Methyl-1,3-butar 123	Sorbitol	58	0.169	-0.355	12.555	0.397	73	68	82	49	35	135	original
11813	16 [644; 2-Methyl-1,3-butar 15	Alanine	64	0.153	0.257	8.423	0.655	74	67	74	67	9	27	duplicate
2043	16 [644; 2-Methyl-1,3-butar 64	[789; Tyramine (3TMS)]	63	0.137	0.221	17.012	0.486	75	66	75	66	66	104	original
2090	16 [644; 2-Methyl-1,3-butar 111	[583; Erythritol (4TMS)]	42	0.080	0.281	31.563	0.434	76	65	73	68	137	129	original
2058	16 [644; 2-Methyl-1,3-butar 79	Glucose	64	0.076	0.467	19.340	0.592	77	64	65	76	82	59	original
2012	16 [644; 2-Methyl-1,3-butar 133	[855; Squalene]	64	0.017	-0.063	16.193	0.439	78	63	85	56	58	127	original
2032	16 [644; 2-Methyl-1,3-butar 53	Glycerol-2-phosphate	64	0.015	-0.034	23.808	0.425	79	62	83	58	109	131	original
2119	16 [644; 2-Methyl-1,3-butar 140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	49	-0.002	0.184	26.392	0.494	80	61	79	62	120	106	original
2069	16 [644; 2-Methyl-1,3-butar 90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	64	-0.011	0.009	14.565	0.439	81	60	82	59	47	128	original
2088	16 [644; 2-Methyl-1,3-butar 109	Oxalacetic acid	64	-0.023	0.299	12.849	0.556	82	59	72	69	38	74	original
2042	16 [644; 2-Methyl-1,3-butar 63	Glutamine	52	-0.030	-0.663	26.383	0.698	83	58	112	29	119	9	original
2097	16 [644; 2-Methyl-1,3-butar 118	[828; Glucopyranose-6-phosphate (6TMS)]	58	-0.044	0.095	20.025	0.441	84	57	80	61	89	123	original
2073	16 [644; 2-Methyl-1,3-butar 94	Hexadecanoic acid	64	-0.078	0.204	10.213	0.571	85	56	78	63	22	67	original
2120	16 [644; 2-Methyl-1,3-butar 141	Lanosta-8,24-dien-3-ol	61	-0.111	0.048	25.929	0.519	86	55	81	60	117	93	original
2051	16 [644; 2-Methyl-1,3-butar 72	[919; D-Xylopyranose (4TMS)]	63	-0.120	-0.197	20.567	0.335	87	54	88	53	94	139	original
2031	16 [644; 2-Methyl-1,3-butar 52	[NA]	46	-0.154	-0.562	30.638	0.680	88	53	101	40	135	17	original
2117	16 [644; 2-Methyl-1,3-butar 138	[874; Ergosterol (1TMS)]	46	-0.159	-0.051	27.514	0.515	89	52	84	57	123	85	original
2118	16 [644; 2-Methyl-1,3-butar 139	[700; Ergosta-5,7-dien-3-ol]	38	-0.164	-0.206	28.370	0.450	90	51	89	52	125	121	original
2050	16 [644; 2-Methyl-1,3-butar 71	[731; Erythrose (3TMS)]	64	-0.165	-0.274	9.303	0.491	91	50	91	50	15	107	original
2086	16 [644; 2-Methyl-1,3-butar 107	9-(Z)-Octadecenoic acid	64	-0.174	-0.262	8.776	0.439	92	49	90	51	13	126	original
2116	16 [644; 2-Methyl-1,3-butar 137	Ergosterol	64	-0.177	-0.183	13.553	0.480	93	48	87	54	41	111	original
2088	16 [644; 2-Methyl-1,3-butar 119	[931; myo-Inositol-2-phosphate (7TMS)]	64	-0.199	-0.131	15.659	0.523	94	47	86	55	53	91	original
2022	16 [644; 2-Methyl-1,3-butar 43	[548; Leucine (2TMS)]	60	-0.203	-0.414	14.703	0.466	95	48	95	45	48	116	original
2047	16 [644; 2-Methyl-1,3-butar 68	[570; Hypoxanthine (2TMS)]	20	-0.221	-0.904	21.031	0.633	96	45	137	4	98	38	original
2004	16 [644; 2-Methyl-1,3-butar 25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.227	-0.890	26.888	0.621	97	44	134	7	121	46	original
10372	16 [644; 2-Methyl-1,3-butar 4	Phosphoric acid	51	-0.230	-0.498	21.365	0.337	98	43	97	44	100	138	duplicate
2040	16 [644; 2-Methyl-1,3-butar 61	[NA]	64	-0.265	-0.392	16.528	0.483	99	42	94	47	62	108	original
2103	16 [644; 2-Methyl-1,3-butar 124	[734; 1-Monoocteoylethanol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	59	-0.266	-0.390	36.433	0.447	100	41	93	48	140	122	original
2109	16 [644; 2-Methyl-1,3-butar 130	Trehalose	63	-0.273	-0.408	15.508	0.385	101	40	95	46	51	139	original
2077	16 [644; 2-Methyl-1,3-butar 98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	48	-0.275	-0.772	30.080	0.603	102	39	123	18	132	52	original
2002	16 [644; 2-Methyl-1,3-butar 23	Homoserine	64	-0.327	-0.850	19.547	0.622	103	38	126	13	86	44	original
2037	16 [644; 2-Methyl-1,3-butar 58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	-0.329	-0.512	12.418	0.425	104	37	99	42	33	132	original
10777	16 [644; 2-Methyl-1,3-butar 7	Threonine	64	-0.333	-0.587	16.192	0.453	105	36	104	37	57	119	duplicate
2068	16 [644; 2-Methyl-1,3-butar 27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	-0.343	-0.833	29.543	0.571	106	35	129	12	130	68	original
2088	16 [644; 2-Methyl-1,3-butar 89	[775; Dopamine (4TMS)]	35	-0.345	-0.762	23.802	0.594	107	34	124	17	108	58	original
2087	16 [644; 2-Methyl-1,3-butar 108	Octadecanoic acid	64	-0.359	-0.518	20.074	0.407	108	33	100	41	91	134	original
2054	16 [644; 2-Methyl-1,3-butar 75	Lysine	64	-0.362	-0.620	25.466	0.468	109	32	105	38	114	115	original
2024	16 [644; 2-Methyl-1,3-butar 45	Homocysteine	61	-0.381	-0.585	34.609	0.440	110	31	103	38	139	124	original
2115	16 [644; 2-Methyl-1,3-butar 136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.382	-0.503	10.140	0.439	111	30	98	43	21	125	original

2015	16 [644; 2-Methyl-1,3-butar	36	[596; N-Acetylglutamic acid (2TMS)]	64	-0.391	-0.635	16,605	0.463	112	29	108	33	63	118 original
10097	16 [644; 2-Methyl-1,3-butar	2	Serine	62	-0.394	-0.688	18,954	0.481	113	28	115	26	79	110 duplicate
2045	16 [644; 2-Methyl-1,3-butar	66	Glyceric acid-3-phosphate	64	-0.398	-0.677	19,469	0.516	114	27	114	27	83	94 original
10910	16 [644; 2-Methyl-1,3-butar	8	Isoleucine	55	-0.414	-0.621	16,692	0.378	115	26	106	35	64	137 duplicate
2028	16 [644; 2-Methyl-1,3-butar	49	[877; Pyrophosphoric acid (4TMS)]	64	-0.448	-0.575	33,470	0.506	116	25	102	39	138	101 original
2010	16 [644; 2-Methyl-1,3-butar	31	[622; Parabanic acid (2TMS)]	64	-0.449	-0.740	24,264	0.524	117	24	118	23	110	90 original
2039	16 [644; 2-Methyl-1,3-butar	60	Glycerol-3-phosphate	64	-0.461	-0.628	10,652	0.539	118	23	107	34	24	84 original
2016	16 [644; 2-Methyl-1,3-butar	37	Phenylalanine	64	-0.470	-0.723	10,657	0.513	119	22	116	25	25	96 original
2074	16 [644; 2-Methyl-1,3-butar	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	-0.478	-0.638	30,521	0.553	120	21	109	32	134	79 original
2027	16 [644; 2-Methyl-1,3-butar	48	Asparagine	64	-0.479	-0.798	20,778	0.639	121	20	125	16	96	35 original
2013	16 [644; 2-Methyl-1,3-butar	34	Aspartic acid	64	-0.484	-0.663	20,245	0.509	122	19	113	28	92	98 original
2046	16 [644; 2-Methyl-1,3-butar	67	Citric acid	64	-0.495	-0.645	10,678	0.452	123	18	111	30	26	120 original
11042	16 [644; 2-Methyl-1,3-butar	9	Proline	63	-0.495	-0.728	22,073	0.474	124	17	117	24	103	114 duplicate
2110	16 [644; 2-Methyl-1,3-butar	131	[626; 5-Methylthioadenosine (3TMS)]	55	-0.503	-0.643	28,533	0.628	125	16	110	31	126	42 original
2012	16 [644; 2-Methyl-1,3-butar	33	Methionine	64	-0.523	-0.747	19,485	0.529	126	15	119	22	84	87 original
2030	16 [644; 2-Methyl-1,3-butar	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.537	-0.830	28,891	0.527	127	14	127	14	128	88 original
2034	16 [644; 2-Methyl-1,3-butar	55	[612; 4-Aminobutyric acid (2TBS)]	43	-0.546	-0.763	30,393	0.591	128	13	121	20	133	60 original
10508	16 [644; 2-Methyl-1,3-butar	5	Leucine	45	-0.556	-0.862	18,333	0.556	129	12	131	10	74	75 duplicate
2009	16 [644; 2-Methyl-1,3-butar	30	[815; Ethyl-3-(2H)-thiophenone]	64	-0.570	-0.756	20,028	0.483	130	11	120	21	90	109 original
2011	16 [644; 2-Methyl-1,3-butar	32	[729; N,N-Dimethyllysine methyl ester]	63	-0.609	-0.894	28,716	0.649	131	10	135	6	127	28 original
10235	16 [644; 2-Methyl-1,3-butar	3	Ethanolamine	62	-0.630	-0.827	24,469	0.595	132	9	126	15	111	57 duplicate
2048	16 [644; 2-Methyl-1,3-butar	69	Arginine	60	-0.640	-0.929	17,485	0.627	133	8	138	3	71	41 original
2038	16 [644; 2-Methyl-1,3-butar	59	Ornithine; Arginine	64	-0.664	-0.771	26,932	0.625	134	7	122	19	122	89 original
11173	16 [644; 2-Methyl-1,3-butar	10	Glycine	64	-0.672	-0.934	14,300	0.691	135	6	139	2	45	12 duplicate
2056	16 [644; 2-Methyl-1,3-butar	77	[826; beta-[[[5-methyl-2-thienyl]methyl]eneamino- benzeneacetic acid methyl ester]	62	-0.683	-0.856	21,908	0.539	136	5	130	11	101	85 original
1999	16 [644; 2-Methyl-1,3-butar	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.712	-0.889	21,033	0.657	137	4	133	8	99	26 original
2060	16 [644; 2-Methyl-1,3-butar	81	Tyrosine	64	-0.722	-0.898	23,267	0.683	138	3	136	5	106	16 original
2021	16 [644; 2-Methyl-1,3-butar	42	Glutamic acid	60	-0.737	-0.868	23,783	0.532	139	2	132	9	107	86 original
2061	16 [644; 2-Methyl-1,3-butar	82	Lysine	39	-0.752	-0.961	16,424	0.654	140	1	140	1	60	28 original
11939	17 [700; 2-methyl-1,2-prop	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	0.840	0.948	2,832	0.645	1	140	2	139	1	2 duplicate
2127	17 [700; 2-methyl-1,2-prop	24	[725; 2-Ketooctanoic acid (2TMS)]	64	0.832	0.949	15,738	0.629	2	139	1	140	52	3 original
2149	17 [700; 2-methyl-1,2-prop	46	Arabinose	64	0.794	0.938	10,024	0.616	3	138	3	138	18	9 original
11561	17 [700; 2-methyl-1,2-prop	13	Uracil	64	0.791	0.932	3,857	0.618	4	137	7	134	2	8 duplicate
2168	17 [700; 2-methyl-1,2-prop	65	[646; 3-Deoxyglucitol (5TMS)]	63	0.784	0.932	18,505	0.628	5	136	6	135	76	5 original
2160	17 [700; 2-methyl-1,2-prop		[757; 2-Desoxy-pentos-3-yose dimethoxyamine (2TMS)]	55	0.779	0.910	13,138	0.603	6	135	15	126	38	15 original
2132	17 [700; 2-methyl-1,2-prop	29	Erythritol	64	0.776	0.931	15,513	0.615	7	134	8	133	50	11 original
2159	17 [700; 2-methyl-1,2-prop	56	[829; Orotic acid (3TMS)]	64	0.774	0.937	17,985	0.628	8	133	5	136	73	4 original
2237	17 [700; 2-methyl-1,2-prop	134	Isomaltose	64	0.763	0.928	9,493	0.615	9	132	9	132	15	10 original
2232	17 [700; 2-methyl-1,2-prop	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	0.762	0.926	15,819	0.590	10	131	10	131	53	24 original
2189	17 [700; 2-methyl-1,2-prop	86	[793; D-Galactono-1,4-lactone (4TMS)]	61	0.760	0.917	12,583	0.594	11	130	12	129	35	21 original
2142	17 [700; 2-methyl-1,2-prop	39	[828; 1-Phenylethanol (1TMS)]	63	0.748	0.916	8,150	0.603	12	129	13	128	7	16 original
2153	17 [700; 2-methyl-1,2-prop	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	0.714	0.910	30,570	0.614	13	128	14	127	136	12 original
11304	17 [700; 2-methyl-1,2-prop	11	Succinic acid	64	0.713	0.895	11,534	0.592	14	127	16	125	25	23 duplicate
2157	17 [700; 2-methyl-1,2-prop	54	[NA]	55	0.701	0.886	21,649	0.542	15	128	17	124	100	53 original
2191	17 [700; 2-methyl-1,2-prop	88	Gluconic acid	64	0.700	0.880	9,185	0.597	16	125	18	123	13	19 original
2141	17 [700; 2-methyl-1,2-prop	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.688	0.918	11,596	0.593	17	124	11	130	27	22 original
2202	17 [700; 2-methyl-1,2-prop	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	0.661	0.938	20,340	0.656	18	123	4	137	91	1 original

2165	17 [700; 2-methyl-1,2-prop	62	[812; D-Xylofuranose (4TMS)]	84	0.861	0.861	5.826	0.552	19	122	20	121	4	47 original
11433	17 [700; 2-methyl-1,2-prop	12	Glyceric acid	63	0.825	0.846	22,721	0.518	20	121	23	118	103	60 duplicate
2168	17 [700; 2-methyl-1,2-prop	103	[648; Ethylamine (2TMS)]	63	0.616	0.821	12,993	0.537	21	120	26	115	37	58 original
11698	17 [700; 2-methyl-1,2-prop	14	Fumaric acid	64	0.598	0.863	20,616	0.566	22	119	18	122	98	36 duplicate
2195	17 [700; 2-methyl-1,2-prop	92	[680; Glycerol-2-phosphate (4TMS)]	54	0.575	0.749	16,106	0.497	23	118	36	105	55	71 original
2176	17 [700; 2-methyl-1,2-prop	73	[708; Glucose methoxyamine (5TMS)]	57	0.566	0.740	16,761	0.486	24	117	37	104	61	78 original
2208	17 [700; 2-methyl-1,2-prop	105	[705; 2-Ketogluconic acid (5TMS)]	48	0.559	0.804	12,949	0.581	25	116	28	113	36	41 original
2125	17 [700; 2-methyl-1,2-prop	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.558	0.848	22,469	0.557	26	115	22	119	101	44 original
2131	17 [700; 2-methyl-1,2-prop	28	Malic acid	64	0.553	0.856	9,920	0.566	27	113	21	120	17	37 original
2179	17 [700; 2-methyl-1,2-prop	76	Fructose	64	0.553	0.844	9,854	0.560	28	114	24	117	16	42 original
2200	17 [700; 2-methyl-1,2-prop	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	0.537	0.765	11,749	0.562	29	112	34	107	28	39 original
2228	17 [700; 2-methyl-1,2-prop	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru	64	0.534	0.783	16,082	0.547	30	111	32	109	54	49 original
2173	17 [700; 2-methyl-1,2-prop	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	0.530	0.559	7,435	0.468	31	110	58	83	6	85 original
2204	17 [700; 2-methyl-1,2-prop	101	[832; Dopamine (4TMS)]	64	0.529	0.730	13,543	0.505	32	109	41	100	40	66 original
2181	17 [700; 2-methyl-1,2-prop	78	Mannose	62	0.525	0.761	18,944	0.485	33	108	35	106	80	75 original
9959	17 [700; 2-methyl-1,2-prop	1	[938; Sulfuric acid (2TMS)]	36	0.514	0.648	16,990	0.600	34	107	52	89	64	17 duplicate
2138	17 [700; 2-methyl-1,2-prop	35	Pyroglutamic acid	64	0.513	0.832	25,859	0.541	35	105	25	116	114	54 original
2143	17 [700; 2-methyl-1,2-prop	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.513	0.787	19,831	0.556	36	106	30	111	85	46 original
2124	17 [700; 2-methyl-1,2-prop	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	0.500	0.727	5,710	0.492	37	104	42	99	3	76 original
2209	17 [700; 2-methyl-1,2-prop	106	[733; Threitol (4TMS)]	62	0.491	0.798	12,311	0.580	38	103	29	112	33	26 original
2194	17 [700; 2-methyl-1,2-prop	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	0.489	0.878	16,591	0.468	39	102	48	93	59	88 original
2218	17 [700; 2-methyl-1,2-prop	15	Glucose-6-phosphate	62	0.484	0.816	9,132	0.573	40	101	27	114	12	30 original
2129	17 [700; 2-methyl-1,2-prop	25	Citramalic acid	64	0.481	0.731	6,756	0.461	41	100	40	101	5	90 original
2190	17 [700; 2-methyl-1,2-prop	87	[945; beta-D-Glucopyranose (5TMS)]	62	0.435	0.696	20,163	0.502	42	99	47	94	89	67 original
10644	17 [700; 2-methyl-1,2-prop	6	Glycerol	64	0.433	0.716	26,820	0.492	43	98	44	97	119	77 duplicate
2203	17 [700; 2-methyl-1,2-prop	100	[857; Mannitol (6TMS)]	64	0.401	0.722	10,778	0.497	44	97	43	98	23	70 original
2223	17 [700; 2-methyl-1,2-prop	120	[945; Uridine (3TMS)]	54	0.398	0.358	8,870	0.575	45	96	70	71	10	28 original
2215	17 [700; 2-methyl-1,2-prop	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.394	0.641	29,168	0.475	46	95	53	88	129	83 original
2205	17 [700; 2-methyl-1,2-prop	102	[904; Galactose methoxyamine (5TMS)]	64	0.377	0.639	17,859	0.498	47	94	54	87	71	69 original
2224	17 [700; 2-methyl-1,2-prop	121	[657; Erythritol (4TMS)]	55	0.372	0.659	25,398	0.545	48	93	50	91	113	50 original
2220	17 [700; 2-methyl-1,2-prop	117	[724; Glycerol (3TMS)]	56	0.371	0.704	12,109	0.562	49	92	46	95	65	38 original
2231	17 [700; 2-methyl-1,2-prop	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.360	0.784	12,109	0.541	50	91	31	110	29	55 original
2213	17 [700; 2-methyl-1,2-prop	110	[715; Erythritol (4TMS)]	54	0.358	0.733	20,357	0.600	51	90	39	102	92	18 original
2225	17 [700; 2-methyl-1,2-prop	122	[844; Erythritol (4TMS)]	52	0.329	0.736	26,129	0.543	52	89	38	103	117	51 original
2121	17 [700; 2-methyl-1,2-prop	18	[590; 1-Acetyl-2-thiohydantoin]	64	0.325	0.533	12,538	0.397	53	88	60	81	34	120 original
2238	17 [700; 2-methyl-1,2-prop	135	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	0.320	0.513	8,664	0.418	54	87	62	79	9	113 original
2216	17 [700; 2-methyl-1,2-prop	113	Galactose-6-phosphate	62	0.305	0.707	18,516	0.522	55	86	45	96	77	59 original
2183	17 [700; 2-methyl-1,2-prop	80	[772; D-Glucose (5TMS)]	62	0.301	0.585	16,405	0.444	56	85	56	85	58	102 original
2147	17 [700; 2-methyl-1,2-prop	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	0.290	0.657	14,262	0.556	57	84	51	90	44	45 original
2188	17 [700; 2-methyl-1,2-prop	85	[529; Methylcitric acid (4TMS)]	48	0.282	0.561	11,127	0.396	58	83	57	84	24	121 original
2235	17 [700; 2-methyl-1,2-prop	132	[895; Isomalbise methoxyamine (8TMS)]	42	0.275	0.766	24,686	0.562	59	82	33	108	111	40 original
2122	17 [700; 2-methyl-1,2-prop	19	Alanine (BP) (3TMS)	64	0.254	0.551	9,358	0.480	60	81	59	82	14	81 original
2217	17 [700; 2-methyl-1,2-prop	114	Fructose-6-phosphate	53	0.231	0.668	19,464	0.570	61	80	49	92	81	34 original
2150	17 [700; 2-methyl-1,2-prop	47	[NA]	64	0.218	0.231	17,371	0.445	62	79	75	66	66	101 original
2207	17 [700; 2-methyl-1,2-prop	104	[795; Erythritol (4TMS)]	63	0.218	0.420	15,428	0.496	63	78	66	75	48	74 original
2219	17 [700; 2-methyl-1,2-prop	116	[882; Psaloudine (5TMS)]	30	0.209	0.383	14,020	0.351	64	77	67	74	43	136 original
2177	17 [700; 2-methyl-1,2-prop	74	[912; Tetradecanoic acid (1TMS)]	64	0.201	0.478	18,319	0.454	65	76	64	77	74	94 original
2199	17 [700; 2-methyl-1,2-prop	96	myo-Inositol	49	0.194	0.207	29,453	0.304	66	75	77	64	131	140 original
2144	17 [700; 2-methyl-1,2-prop	41	[639; Proline (2TMS)]	64	0.188	0.377	8,501	0.431	67	74	68	73	8	108 original
2230	17 [700; 2-methyl-1,2-prop	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.185	0.593	15,226	0.575	68	73	55	88	48	29 original

2187	17 [700; 2-methyl-1,2-propyl]	84	Mannitol	62	0.166	0.511	17.600	0.494	69	72	63	78	70	79	original
2226	17 [700; 2-methyl-1,2-propyl]	123	[945; Galactofuranose-6-phosphate (7TMS)]	64	0.163	0.374	10.052	0.513	70	71	69	72	20	61	original
2186	17 [700; 2-methyl-1,2-propyl]	93	[607; Putrescine (4TMS)]	60	0.159	0.323	28.010	0.405	71	70	72	68	123	116	original
2229	17 [700; 2-methyl-1,2-propyl]	126	[559; Erythritol (4TMS)]	45	0.152	0.458	18.744	0.582	72	69	65	76	79	25	original
2186	17 [700; 2-methyl-1,2-propyl]	83	Sorbitol	58	0.147	-0.301	13.592	0.378	73	68	90	51	41	131	original
2181	17 [700; 2-methyl-1,2-propyl]	15	Alanine	64	0.138	0.330	8.890	0.568	74	67	71	70	11	35	duplicate
2167	17 [700; 2-methyl-1,2-propyl]	64	[789; Tyramine (3TMS)]	63	0.131	0.277	16.897	0.384	75	68	73	68	62	127	original
2182	17 [700; 2-methyl-1,2-propyl]	79	Glucose	64	0.083	0.521	20.042	0.539	76	65	61	80	88	56	original
2156	17 [700; 2-methyl-1,2-propyl]	53	Glycerol-2-phosphate	64	0.026	-0.057	23.628	0.350	77	84	82	59	106	137	original
2214	17 [700; 2-methyl-1,2-propyl]	111	[583; Erythritol (4TMS)]	42	0.001	0.217	31.730	0.369	78	63	76	65	137	124	original
2221	17 [700; 2-methyl-1,2-propyl]	118	[928; Glucopyranose-6-phosphate (6TMS)]	58	0.001	0.150	19.850	0.443	79	62	78	63	86	103	original
2236	17 [700; 2-methyl-1,2-propyl]	133	[855; Squalene]	64	0.000	-0.049	18.300	0.368	80	61	81	60	57	132	original
2193	17 [700; 2-methyl-1,2-propyl]	90	[910; 9-(Z)-Hexadecanoic acid (1TMS)]	64	-0.028	-0.086	14.930	0.384	81	60	84	57	46	128	original
2243	17 [700; 2-methyl-1,2-propyl]	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	49	-0.053	0.068	26.083	0.380	82	59	80	61	116	130	original
2166	17 [700; 2-methyl-1,2-propyl]	63	Glutamine	52	-0.053	-0.659	26.846	0.621	83	58	117	24	120	7	original
2212	17 [700; 2-methyl-1,2-propyl]	109	Octadecanoic acid	64	-0.052	0.255	13.686	0.436	84	57	74	67	42	106	original
2175	17 [700; 2-methyl-1,2-propyl]	72	[919; D-Xylopyranose (4TMS)]	63	-0.083	-0.184	20.549	0.325	85	56	86	55	94	138	original
2197	17 [700; 2-methyl-1,2-propyl]	94	Hexadecanoic acid	64	-0.092	0.149	11.535	0.448	86	55	79	62	26	99	original
2244	17 [700; 2-methyl-1,2-propyl]	141	Lanosta-8,24-dien-3-beta-ol	61	-0.168	-0.084	25.899	0.421	87	54	83	58	115	112	original
2210	17 [700; 2-methyl-1,2-propyl]	107	9-(Z)-Octadecenoic acid	64	-0.181	-0.332	10.049	0.365	88	53	91	50	19	133	original
2146	17 [700; 2-methyl-1,2-propyl]	43	[548; Leucine (2TBS)]	60	-0.193	-0.356	14.942	0.414	89	52	93	48	47	114	original
2155	17 [700; 2-methyl-1,2-propyl]	52	[NA]	46	-0.194	-0.581	30.546	0.608	90	51	106	35	135	14	original
2174	17 [700; 2-methyl-1,2-propyl]	4	Phosphoric acid	64	-0.199	-0.284	10.118	0.389	91	50	89	52	21	123	original
10373	17 [700; 2-methyl-1,2-propyl]	4	Ergosterol	51	-0.206	-0.428	22.517	0.318	92	49	96	45	102	139	duplicate
2242	17 [700; 2-methyl-1,2-propyl]	139	[700; Ergosta-5,7-dien-3-ol]	38	-0.209	-0.335	28.347	0.380	93	48	92	49	125	129	original
2128	17 [700; 2-methyl-1,2-propyl]	25	[709; 2,5-Diaminvalerolactam (2TMS)]	48	-0.216	-0.802	26.838	0.571	94	47	131	10	121	31	original
2222	17 [700; 2-methyl-1,2-propyl]	119	[931; myo-Inositol-2-phosphate (7TMS)]	64	-0.218	-0.211	16.106	0.399	95	48	88	53	56	119	original
2240	17 [700; 2-methyl-1,2-propyl]	137	Ergosterol	64	-0.221	-0.205	14.323	0.363	96	45	87	54	45	134	original
2241	17 [700; 2-methyl-1,2-propyl]	138	[874; Ergosterol (1TMS)]	46	-0.229	-0.104	27.416	0.447	97	44	85	56	122	100	original
2201	17 [700; 2-methyl-1,2-propyl]	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	48	-0.239	-0.678	29.885	0.483	98	43	119	22	132	80	original
2164	17 [700; 2-methyl-1,2-propyl]	61	[NA]	64	-0.270	-0.399	16.711	0.467	99	42	95	46	60	87	original
2233	17 [700; 2-methyl-1,2-propyl]	130	Trehalose	63	-0.273	-0.456	16.904	0.388	100	41	98	43	63	125	original
2171	17 [700; 2-methyl-1,2-propyl]	68	[570; Hypoxanthine (2TMS)]	20	-0.274	-0.892	20.605	0.570	101	40	139	2	95	33	original
2227	17 [700; 2-methyl-1,2-propyl]	124	[734; 1-Monodeoxyglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	59	-0.285	-0.460	36.209	0.387	102	39	99	42	140	126	original
2161	17 [700; 2-methyl-1,2-propyl]	58	[636; 4R-Acetylaminido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexene (1TMS)]	64	-0.305	-0.455	13.278	0.404	103	38	97	44	39	118	original
2130	17 [700; 2-methyl-1,2-propyl]	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	-0.315	-0.748	29.442	0.499	104	37	124	17	130	68	original
2239	17 [700; 2-methyl-1,2-propyl]	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.324	-0.387	10.147	0.436	105	36	94	47	22	105	original
2126	17 [700; 2-methyl-1,2-propyl]	23	Homoserine	64	-0.332	-0.770	19.922	0.551	106	35	127	14	87	48	original
2192	17 [700; 2-methyl-1,2-propyl]	89	[775; Dopamine (4TMS)]	35	-0.338	-0.779	23.851	0.509	107	34	129	12	107	63	original
10778	17 [700; 2-methyl-1,2-propyl]	7	Threonine	64	-0.352	-0.545	17.480	0.431	108	33	103	38	67	109	duplicate
2178	17 [700; 2-methyl-1,2-propyl]	75	Lysine	64	-0.355	-0.571	26.603	0.456	109	32	105	36	118	93	original
2148	17 [700; 2-methyl-1,2-propyl]	45	Homocysteine	61	-0.363	-0.520	34.285	0.424	110	31	100	41	139	111	original
2211	17 [700; 2-methyl-1,2-propyl]	108	Octadecanoic acid	64	-0.364	-0.540	20.215	0.395	111	30	102	39	90	122	original
2139	17 [700; 2-methyl-1,2-propyl]	36	[596; N-Acetylglutamic acid (2TMS)]	64	-0.396	-0.595	17.921	0.436	112	29	108	33	72	107	original
10098	17 [700; 2-methyl-1,2-propyl]	2	Serine	62	-0.398	-0.613	19.671	0.453	113	28	109	32	83	95	duplicate
2152	17 [700; 2-methyl-1,2-propyl]	49	[877; Pyrophosphoric acid (4TMS)]	64	-0.404	-0.525	33.331	0.426	114	27	101	40	138	110	original
2169	17 [700; 2-methyl-1,2-propyl]	66	Glycercic acid-3-phosphate	64	-0.409	-0.613	19.486	0.458	115	26	110	31	82	91	original
10911	17 [700; 2-methyl-1,2-propyl]	8	Isoleucine	55	-0.420	-0.557	17.566	0.358	116	25	104	37	69	135	duplicate
2134	17 [700; 2-methyl-1,2-propyl]	31	[622; Parabanic acid (2TMS)]	64	-0.433	-0.659	24.175	0.464	117	24	115	26	108	88	original



2151	17 [700; 2-methyl-1,2-propyl]	48	Asparagine	64	-0.452	-0.771	21,326	0.596	118	23	128	13	98	20 original
2137	17 [700; 2-methyl-1,2-propyl]	34	Aspartic acid	64	-0.457	-0.587	21,408	0.463	119	22	107	34	99	89 original
2163	17 [700; 2-methyl-1,2-propyl]	60	Glycerol-3-phosphate	64	-0.466	-0.619	12,163	0.451	120	21	111	30	31	96 original
2140	17 [700; 2-methyl-1,2-propyl]	37	Phenylalanine	64	-0.477	-0.682	12,140	0.471	121	20	120	21	30	84 original
2198	17 [700; 2-methyl-1,2-propyl]	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	-0.478	-0.645	30,434	0.410	122	19	114	27	134	115 original
2234	17 [700; 2-methyl-1,2-propyl]	131	[626; 5-Methylthioadenosine (3TMS)]	55	-0.488	-0.645	28,447	0.509	123	18	113	28	128	62 original
2170	17 [700; 2-methyl-1,2-propyl]	67	Citric acid	64	-0.490	-0.639	12,204	0.405	124	17	112	29	32	117 original
11043	17 [700; 2-methyl-1,2-propyl]	9	Proline	63	-0.493	-0.659	23,112	0.449	125	16	116	25	104	98 duplicate
2136	17 [700; 2-methyl-1,2-propyl]	33	Methionine	64	-0.504	-0.676	19,829	0.480	126	15	118	23	84	82 original
2154	17 [700; 2-methyl-1,2-propyl]	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.535	-0.746	28,567	0.442	127	13	123	16	127	104 original
2158	17 [700; 2-methyl-1,2-propyl]	55	[612; 4-Aminobutyric acid (2BTS)]	43	-0.535	-0.755	30,215	0.505	128	14	126	15	133	65 original
2133	17 [700; 2-methyl-1,2-propyl]	30	[815; Ethyl-3(2H)-thiophenone]	64	-0.563	-0.690	21,233	0.457	129	12	121	20	97	92 original
2135	17 [700; 2-methyl-1,2-propyl]	32	[729; N,N-Dimethyllysine methyl ester]	63	-0.564	-0.816	28,879	0.571	130	11	133	8	128	32 original
10509	17 [700; 2-methyl-1,2-propyl]	5	Leucine	45	-0.568	-0.755	18,366	0.449	131	10	125	16	75	97 duplicate
2172	17 [700; 2-methyl-1,2-propyl]	69	Arginine	60	-0.589	-0.848	18,606	0.576	132	8	135	6	78	27 original
2162	17 [700; 2-methyl-1,2-propyl]	59	Ornithine; Arginine	64	-0.607	-0.708	28,068	0.506	133	8	122	19	124	64 original
10236	17 [700; 2-methyl-1,2-propyl]	3	Ethanolamine	62	-0.613	-0.819	24,632	0.543	134	7	134	7	109	52 duplicate
2180	17 [700; 2-methyl-1,2-propyl]	77	[826; beta-[[5-methyl-2-thienyl)methyl]enearmino-benzeneacetic acid methyl ester]	62	-0.647	-0.809	23,220	0.496	135	6	132	9	105	73 original
2185	17 [700; 2-methyl-1,2-propyl]	82	Lysine	39	-0.652	-0.876	17,545	0.539	136	5	137	4	68	57 original
11174	17 [700; 2-methyl-1,2-propyl]	10	Glycine	64	-0.655	-0.893	15,586	0.609	137	4	140	1	51	13 duplicate
2145	17 [700; 2-methyl-1,2-propyl]	42	Glutamic acid	60	-0.680	-0.795	24,938	0.496	138	3	130	11	112	72 original
2184	17 [700; 2-methyl-1,2-propyl]	81	Tyrosine	64	-0.691	-0.861	24,651	0.621	139	2	136	5	110	6 original
2123	17 [700; 2-methyl-1,2-propyl]	20		31	-0.729	-0.885	20,540	0.559	140	1	138	3	93	43 original
2247	18 [590; 1-Acetyl-2-thiophenyl]	21	[618; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	64	0.726	0.883	10,568	0.550	1	140	1	140	44	1 original
2341	18 [590; 1-Acetyl-2-thiophenyl]	115	Glucose-6-phosphate	62	0.555	0.638	19,363	0.476	2	139	11	130	104	14 original
2252	18 [590; 1-Acetyl-2-thiophenyl]	26	Citramalic acid	64	0.555	0.753	10,753	0.466	3	138	2	139	45	24 original
2254	18 [590; 1-Acetyl-2-thiophenyl]	28	Malic acid	64	0.527	0.685	3,620	0.486	4	137	5	136	2	11 original
2266	18 [590; 1-Acetyl-2-thiophenyl]	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.491	0.700	29,392	0.492	5	136	3	138	133	7 original
2340	18 [590; 1-Acetyl-2-thiophenyl]	114	Fructose-6-phosphate	53	0.491	0.644	9,466	0.429	6	135	9	132	36	63 original
2339	18 [590; 1-Acetyl-2-thiophenyl]	113	Galactose-6-phosphate	62	0.486	0.631	9,007	0.426	7	134	14	127	33	65 original
2351	18 [590; 1-Acetyl-2-thiophenyl]	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	0.482	0.562	26,802	0.420	8	133	32	109	127	71 original
2245	18 [590; 1-Acetyl-2-thiophenyl]	19	Alanine (BP) (3TMS)	64	0.478	0.677	6,486	0.462	9	131	6	135	15	30 original
2326	18 [590; 1-Acetyl-2-thiophenyl]	100	[857; Mannitol (6TMS)]	64	0.478	0.568	3,784	0.431	10	132	30	111	3	56 original
2302	18 [590; 1-Acetyl-2-thiophenyl]	76	Fructose	64	0.465	0.608	20,446	0.449	11	130	21	120	109	42 original
11689	18 [590; 1-Acetyl-2-thiophenyl]	14	Fumaric acid	64	0.463	0.657	9,900	0.466	12	129	8	133	39	26 duplicate
2300	18 [590; 1-Acetyl-2-thiophenyl]	74	[912; Tetradecanoic acid (1TMS)]	64	0.461	0.697	9,261	0.487	13	127	4	137	34	10 original
2261	18 [590; 1-Acetyl-2-thiophenyl]	35	Pyroglutamic acid	62	0.456	0.642	8,153	0.522	15	126	10	131	25	3 original
2332	18 [590; 1-Acetyl-2-thiophenyl]	108	[733; Threitol (4TMS)]	64	0.451	0.669	3,071	0.449	16	125	7	134	1	41 duplicate
11305	18 [590; 1-Acetyl-2-thiophenyl]	11	Succinic acid	64	0.440	0.622	3,839	0.469	17	124	16	125	4	19 original
2264	18 [590; 1-Acetyl-2-thiophenyl]	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.433	0.596	8,466	0.447	18	123	23	118	27	44 original
2268	18 [590; 1-Acetyl-2-thiophenyl]	62	[912; D-Xylofuranose (4TMS)]	55	0.432	0.633	15,019	0.491	19	122	12	129	75	8 original
2347	18 [590; 1-Acetyl-2-thiophenyl]	121	[657; Erythritol (4TMS)]	42	0.431	0.524	16,611	0.431	20	121	45	96	84	59 original
2358	18 [590; 1-Acetyl-2-thiophenyl]	132	[895; Isomaltose methoxyamine (8TMS)]	63	0.427	0.632	18,038	0.435	21	120	13	128	95	53 original
2338	18 [590; 1-Acetyl-2-thiophenyl]	102	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	64	0.417	0.548	6,966	0.432	22	119	37	104	18	55 original
2248	18 [590; 1-Acetyl-2-thiophenyl]	22	[690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.416	0.580	13,293	0.457	23	118	27	114	69	37 original
2270	18 [590; 1-Acetyl-2-thiophenyl]	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	0.416	0.550	8,376	0.463	24	117	35	108	26	29 original
11434	18 [590; 1-Acetyl-2-thiophenyl]	12	Glycetic acid	63	0.415	0.620	12,067	0.457	25	116	17	124	55	36 duplicate
2343	18 [590; 1-Acetyl-2-thiophenyl]	117	[724; Glycerol (3TMS)]	56	0.414	0.615	8,566	0.494	26	115	19	122	28	6 original

2304	18 [590; 1-Acetyl-2-thiohydi]	78	Mannose	62	0.411	0.584	11,310	0.475	27	114	26	115	48	18 original
	135													
2361	18 [590; 1-Acetyl-2-thiohydi]	122	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	0.410	0.609	6,639	0.420	28	113	20	121	16	70 original
2348	18 [590; 1-Acetyl-2-thiohydi]	122	[644; Erythritol (4TMS)]	52	0.409	0.565	16,775	0.511	29	112	31	110	86	5 original
2267	18 [590; 1-Acetyl-2-thiohydi]	41	[639; Proline (2TMS)]	64	0.406	0.623	8,001	0.431	30	111	15	126	24	58 original
2352	18 [590; 1-Acetyl-2-thiohydi]	126	[559; Erythritol (4TMS)]	45	0.402	0.555	8,729	0.511	31	110	33	108	29	4 original
2312	18 [590; 1-Acetyl-2-thiohydi]	86	[783; D-Galactono-1,4-lactone (4TMS)]	61	0.388	0.598	18,763	0.468	32	109	22	119	100	20 original
2309	18 [590; 1-Acetyl-2-thiohydi]	83	Sorbitol	58	0.388	0.151	16,483	0.319	33	108	77	64	81	136 original
2296	18 [590; 1-Acetyl-2-thiohydi]	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	0.380	0.442	13,554	0.397	34	107	54	87	71	87 original
2259	18 [590; 1-Acetyl-2-thiohydi]	29	Erythritol	64	0.379	0.575	5,141	0.460	35	106	28	113	7	32 original
2255	18 [590; 1-Acetyl-2-thiohydi]	73	[708; Glucose methoxyamine (5TMS)]	57	0.368	0.574	10,370	0.408	36	105	29	112	42	82 original
2250	18 [590; 1-Acetyl-2-thiohydi]	24	[725; 2-Ketocacetic acid (2TMS)]	64	0.356	0.553	26,946	0.458	37	104	34	107	129	34 original
2265	18 [590; 1-Acetyl-2-thiohydi]	39	[829; 1-Phenylethanol (1TMS)]	63	0.354	0.545	12,716	0.453	38	103	38	103	62	39 original
2346	18 [590; 1-Acetyl-2-thiohydi]	120	[945; Uridine (3TMS)]	54	0.352	0.314	7,207	0.446	39	102	66	75	21	45 original
11840	18 [590; 1-Acetyl-2-thiohydi]	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	0.350	0.549	12,504	0.465	40	101	38	105	59	28 duplicate
2336	18 [590; 1-Acetyl-2-thiohydi]	110	[715; Erythritol (4TMS)]	54	0.347	0.502	12,791	0.456	41	100	48	93	64	2 original
2342	18 [590; 1-Acetyl-2-thiohydi]	123	[882; Pseudouridine (5TMS)]	30	0.347	0.373	9,362	0.357	42	99	60	81	35	121 original
2319	18 [590; 1-Acetyl-2-thiohydi]	85	[945; Galactofuranose-6-phosphate (7TMS)]	64	0.341	0.519	5,451	0.430	43	98	46	95	8	60 original
2311	18 [590; 1-Acetyl-2-thiohydi]	85	[529; Methylenecitric acid (4TMS)]	48	0.332	0.516	4,176	0.438	44	97	18	123	5	50 original
2314	18 [590; 1-Acetyl-2-thiohydi]	88	Gluconic acid	64	0.331	0.502	8,732	0.428	45	96	49	92	30	64 original
2330	18 [590; 1-Acetyl-2-thiohydi]	104	[785; Erythritol (4TMS)]	63	0.326	0.484	6,442	0.438	46	95	50	91	14	48 original
12064	18 [590; 1-Acetyl-2-thiohydi]	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	0.325	0.533	12,538	0.397	47	94	41	100	60	86 duplicate
2282	18 [590; 1-Acetyl-2-thiohydi]	56	[829; Oroic acid (3TMS)]	64	0.304	0.528	11,877	0.449	48	93	44	97	53	43 original
2322	18 [590; 1-Acetyl-2-thiohydi]	96	myo-Inositol	49	0.303	0.327	20,654	0.279	49	92	64	77	112	139 original
2272	18 [590; 1-Acetyl-2-thiohydi]	46	Arabinose	64	0.302	0.537	14,645	0.446	50	91	40	101	74	46 original
2276	18 [590; 1-Acetyl-2-thiohydi]	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	0.298	0.457	20,397	0.422	51	90	53	88	108	69 original
2291	18 [590; 1-Acetyl-2-thiohydi]	65	[646; 3-Deoxyglucitol (5TMS)]	63	0.297	0.537	14,106	0.443	52	89	39	102	73	47 original
2280	18 [590; 1-Acetyl-2-thiohydi]	54	[NA]	55	0.293	0.458	13,299	0.379	53	88	52	89	70	99 original
11562	18 [590; 1-Acetyl-2-thiohydi]	13	Uracil	64	0.287	0.517	11,532	0.482	54	87	47	94	49	12 duplicate
2360	18 [590; 1-Acetyl-2-thiohydi]	134	Isomaltose	64	0.283	0.531	20,625	0.465	55	86	42	99	111	27 original
10645	18 [590; 1-Acetyl-2-thiohydi]	6	Glycerol	64	0.280	0.424	36,799	0.371	56	85	55	86	140	106 duplicate
2366	18 [590; 1-Acetyl-2-thiohydi]	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	49	0.274	0.338	16,828	0.408	57	84	63	78	87	80 original
2359	18 [590; 1-Acetyl-2-thiohydi]	133	[855; Squalene]	64	0.270	0.326	6,407	0.365	58	83	65	76	12	113 original
2337	18 [590; 1-Acetyl-2-thiohydi]	111	[583; Erythritol (4TMS)]	42	0.264	0.367	21,338	0.377	59	82	61	80	115	101 original
2335	18 [590; 1-Acetyl-2-thiohydi]	109	Octadecanoic acid	64	0.262	0.591	17,401	0.476	60	81	24	117	91	15 original
2364	18 [590; 1-Acetyl-2-thiohydi]	138	[674; Ergosterol (1TMS)]	46	0.262	0.424	17,254	0.364	61	80	56	85	90	115 original
2280	18 [590; 1-Acetyl-2-thiohydi]	64	[789; Tyramine (3TMS)]	63	0.259	0.311	5,878	0.348	62	79	67	74	9	129 original
	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]												
2355	18 [590; 1-Acetyl-2-thiohydi]	94	Hexadecanoic acid	59	0.243	0.460	11,589	0.423	63	78	51	90	50	67 original
2320	18 [590; 1-Acetyl-2-thiohydi]	92	[680; Glycero-2-phosphate (4TMS)]	64	0.225	0.529	16,363	0.451	64	77	43	98	80	40 original
2318	18 [590; 1-Acetyl-2-thiohydi]	103	[648; Ethylamine (2TMS)]	54	0.220	0.394	8,980	0.387	65	76	59	82	32	93 original
2329	18 [590; 1-Acetyl-2-thiohydi]	87	[945; beta-D-Glucopyranose (5TMS)]	63	0.208	0.245	13,214	0.416	66	75	72	69	68	73 original
2313	18 [590; 1-Acetyl-2-thiohydi]	101	[832; Dopamine (4TMS)]	62	0.204	0.365	30,486	0.378	67	74	62	79	136	100 original
	57													
2283	18 [590; 1-Acetyl-2-thiohydi]	71	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55	0.193	0.419	12,659	0.437	68	73	57	84	61	51 original
2297	18 [590; 1-Acetyl-2-thiohydi]	79	[731; Erythrose (3TMS)]	64	0.184	0.276	6,847	0.382	69	72	70	71	17	95 original
2305	18 [590; 1-Acetyl-2-thiohydi]	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.163	0.234	6,149	0.358	71	70	75	66	11	119 original
2353	18 [590; 1-Acetyl-2-thiohydi]	137	Ergosterol	64	0.162	0.244	10,544	0.402	72	69	73	68	43	84 original
2363	18 [590; 1-Acetyl-2-thiohydi]	141	Lanosta-8,24-dien-3-beta-ol	64	0.160	0.143	10,361	0.345	73	68	76	63	41	133 original
2327	18 [590; 1-Acetyl-2-thiohydi]	141		61	0.157	0.216	15,322	0.418	74	67	76	65	76	72 original

11815	18 [590; 1-Acetyl-2-thiohydi]	15 Alanine	64	0.152	0.250	13.664	0.412	75	66	71	70	72	77 duplicate
2354	18 [590; 1-Acetyl-2-thiohydi]	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.147	0.235	7.063	0.398	76	65	74	67	19	92 original
2306	18 [590; 1-Acetyl-2-thiohydi]	80 [772; D-Glucose (5TMS)]	62	0.135	0.307	26.075	0.359	77	64	68	73	125	118 original
2282	18 [590; 1-Acetyl-2-thiohydi]	36 [596; N-Acetylglutamic acid (2TMS)]	64	0.108	0.052	23.861	0.363	78	63	83	58	119	116 original
2365	18 [590; 1-Acetyl-2-thiohydi]	139 [700; Ergosta-5,7-dien-3-ol]	38	0.092	-0.003	19.400	0.274	79	62	87	54	105	140 original
2317	18 [590; 1-Acetyl-2-thiohydi]	95 [766; beta-D-Methylglucopyranoside (4TMS)]	64	0.086	0.073	17.041	0.367	80	61	82	59	89	111 original
2331	18 [590; 1-Acetyl-2-thiohydi]	101 [705; 2-Ketogluconic acid (5TMS)]	48	0.071	0.085	11.264	0.395	81	60	81	60	47	88 original
2310	18 [590; 1-Acetyl-2-thiohydi]	84 Mannitol	62	0.051	0.000	27.547	0.375	82	59	86	55	130	103 original
2344	18 [590; 1-Acetyl-2-thiohydi]	118 [828; Glucopyranose-6-phosphate (6TMS)]	58	0.049	0.102	10.356	0.351	83	58	79	62	40	126 original
2323	18 [590; 1-Acetyl-2-thiohydi]	97 [756; beta-D-Methylglucopyranoside (4TMS)]	52	0.042	0.088	18.420	0.377	84	57	80	61	99	102 original
2345	18 [590; 1-Acetyl-2-thiohydi]	119 [931; myo-Inositol-2-phosphate (7TMS)]	64	0.030	0.032	7.153	0.391	85	56	84	57	20	91 original
		124 [734; 1-Monooleoylglycerol (2TMS); 1-Monoheptadecanoylglycerol (1TMS)]	59	0.027	-0.091	25.201	0.365	86	55	94	47	122	114 original
2350	18 [590; 1-Acetyl-2-thiohydi]	99 [682; Ribose-5-phosphate methoxamine (BP) (5TMS)]	41	0.024	0.293	12.130	0.400	87	54	69	72	56	85 original
2286	18 [590; 1-Acetyl-2-thiohydi]	60 Glycerol-3-phosphate	64	-0.034	0.025	16.517	0.388	88	53	85	56	82	109 original
2333	18 [590; 1-Acetyl-2-thiohydi]	107 9-(Z)-Octadecenoic acid	64	-0.038	-0.096	9.872	0.355	89	52	85	46	38	122 original
2293	18 [590; 1-Acetyl-2-thiohydi]	67 Citric acid	64	-0.044	-0.052	18.779	0.348	90	50	90	51	102	128 original
2316	18 [590; 1-Acetyl-2-thiohydi]	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	64	-0.044	-0.084	6.066	0.375	91	51	92	49	10	104 original
2356	18 [590; 1-Acetyl-2-thiohydi]	130 Trehalose	63	-0.051	-0.105	24.993	0.393	92	49	86	45	121	90 original
2362	18 [590; 1-Acetyl-2-thiohydi]	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.059	-0.120	4.767	0.291	93	48	89	42	6	138 original
		58 [636; 4R-Acetamid-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	-0.064	-0.050	12.149	0.357	94	47	89	52	57	120 original
2284	18 [590; 1-Acetyl-2-thiohydi]	75 Lysine	64	-0.083	-0.090	34.931	0.363	95	46	93	48	137	117 original
2301	18 [590; 1-Acetyl-2-thiohydi]	4 Phosphoric acid	51	-0.095	-0.050	28.933	0.302	96	45	88	53	132	137 duplicate
10374	18 [590; 1-Acetyl-2-thiohydi]	66 Glycine acid-3-phosphate	64	-0.105	-0.117	7.981	0.382	97	44	98	43	23	96 original
2292	18 [590; 1-Acetyl-2-thiohydi]	7 Threonine	64	-0.112	-0.053	25.274	0.366	98	43	91	50	123	112 duplicate
10779	18 [590; 1-Acetyl-2-thiohydi]	108 Octadecenoic acid	64	-0.120	-0.107	8.893	0.348	99	42	97	44	31	130 original
2334	18 [590; 1-Acetyl-2-thiohydi]	47 [NA]	64	-0.121	-0.257	11.873	0.416	100	41	106	35	52	74 original
2273	18 [590; 1-Acetyl-2-thiohydi]	72 [919; D-Xylopyranose (4TMS)]	63	-0.127	-0.194	10.961	0.346	101	40	102	39	46	132 original
2298	18 [590; 1-Acetyl-2-thiohydi]	37 Phenylalanine	64	-0.134	-0.130	17.838	0.348	102	39	100	41	93	127 original
2263	18 [590; 1-Acetyl-2-thiohydi]	53 Glycerol-2-phosphate	64	-0.139	-0.314	12.729	0.347	103	38	109	32	63	131 original
9960	18 [590; 1-Acetyl-2-thiohydi]	1 [938; Sulfuric acid (2TMS)]	36	-0.152	-0.135	9.849	0.435	104	37	101	40	37	52 duplicate
2324	18 [590; 1-Acetyl-2-thiohydi]	98 [697; Ribose-5-phosphate methoxamine (5TMS)]	48	-0.160	-0.349	20.056	0.424	105	36	114	27	106	66 original
2319	18 [590; 1-Acetyl-2-thiohydi]	93 [607; Putrescine (4TMS)]	60	-0.163	-0.253	18.849	0.365	106	35	105	36	103	123 original
10237	18 [590; 1-Acetyl-2-thiohydi]	3 Ethanolamine	62	-0.201	-0.335	13.185	0.404	107	34	112	29	67	83 duplicate
2253	18 [590; 1-Acetyl-2-thiohydi]	27 [815; (E)-4-Methyl-5-hydroxy-3-pentan-2-one (1TMS)]	53	-0.216	-0.579	20.804	0.460	108	33	131	10	113	33 original
2281	18 [590; 1-Acetyl-2-thiohydi]	55 [612; 4-Aminobutyric acid (2TBS)]	43	-0.236	-0.469	23.333	0.380	109	32	121	20	117	97 original
2287	18 [590; 1-Acetyl-2-thiohydi]	61 [NA]	64	-0.238	-0.245	6.424	0.374	110	31	104	37	13	105 original
10099	18 [590; 1-Acetyl-2-thiohydi]	2 Serine	62	-0.243	-0.205	16.872	0.351	111	30	103	38	88	125 duplicate
2307	18 [590; 1-Acetyl-2-thiohydi]	81 Tyrosine	64	-0.245	-0.315	29.919	0.438	112	29	110	31	135	49 original
2277	18 [590; 1-Acetyl-2-thiohydi]	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.254	-0.321	20.494	0.385	113	28	111	30	110	94 original
2258	18 [590; 1-Acetyl-2-thiohydi]	32 [729; N,N-Dimethyllysine methyl ester]	63	-0.260	-0.398	18.287	0.466	114	27	117	24	98	25 original
2278	18 [590; 1-Acetyl-2-thiohydi]	77 [826; beta-[(5-methyl-2-thienyl)methyl]eneamino-benzeneacetic acid methyl ester]	46	-0.287	-0.484	20.870	0.431	115	26	123	18	114	57 original
		59 Ornithine; Arginine	62	-0.300	-0.378	26.253	0.395	116	25	115	26	126	89 original
2303	18 [590; 1-Acetyl-2-thiohydi]	10 Glycine	64	-0.308	-0.338	36.349	0.371	117	24	113	28	139	107 original
11175	18 [590; 1-Acetyl-2-thiohydi]	43 [548; Leucine (2TBS)]	60	-0.338	-0.533	7.670	0.408	119	22	125	16	22	79 original
2269	18 [590; 1-Acetyl-2-thiohydi]	31 [622; Parabenic acid (2TMS)]	64	-0.339	-0.446	12.921	0.407	120	21	119	22	65	81 original
2257	18 [590; 1-Acetyl-2-thiohydi]	131 [628; 5-Methylthiadenosine (3TMS)]	55	-0.340	-0.562	18.104	0.476	121	20	129	12	96	16 original
2295	18 [590; 1-Acetyl-2-thiohydi]	69 Arginine	60	-0.341	-0.563	18.775	0.467	122	19	130	11	101	23 original

2274	18 [590; 1-Acetyl-2-thiocydi]	48	Asparagine	64	-0.343	-0.555	13.043	0.416	123	18	128	13	66	75 original
2284	18 [590; 1-Acetyl-2-thiocydi]	68	[570; Hypoxanthine (2TMS)]	20	-0.347	-0.631	15.463	0.411	124	17	136	5	77	78 original
11044	18 [590; 1-Acetyl-2-thiocydi]	9	Proline	63	-0.358	-0.265	24.573	0.367	125	16	107	34	120	110 duplicate
2289	18 [590; 1-Acetyl-2-thiocydi]	63	Glutamine	52	-0.359	-0.493	17.961	0.370	126	15	124	17	94	108 original
2288	18 [590; 1-Acetyl-2-thiocydi]	42	Glutamic acid	60	-0.360	-0.385	26.887	0.351	127	14	116	25	128	124 original
10912	18 [590; 1-Acetyl-2-thiocydi]	8	Isoleucine	55	-0.370	-0.282	16.576	0.340	128	13	108	33	83	134 duplicate
2256	18 [590; 1-Acetyl-2-thiocydi]	30	[815; Ethyl-3(2H)-thiophenone]	64	-0.373	-0.404	26.070	0.380	129	12	118	23	124	98 original
2259	18 [590; 1-Acetyl-2-thiocydi]	33	Methionine	64	-0.375	-0.473	11.673	0.434	130	11	122	19	51	54 original
2321	18 [590; 1-Acetyl-2-thiocydi]	95	[770; 3,4,6-Trisubstitutedphenylmethanamine (5TMS)]	50	-0.376	-0.541	20.268	0.477	131	10	127	14	107	13 original
2260	18 [590; 1-Acetyl-2-thiocydi]	34	Aspartic acid	64	-0.378	-0.455	28.536	0.429	132	9	120	21	131	62 original
2249	18 [590; 1-Acetyl-2-thiocydi]	23	Homoserine	64	-0.396	-0.623	11.917	0.455	133	8	135	6	54	38 original
2315	18 [590; 1-Acetyl-2-thiocydi]	89	[775; Dopamine (4TMS)]	35	-0.412	-0.594	18.118	0.339	134	7	133	8	97	135 original
2271	18 [590; 1-Acetyl-2-thiocydi]	45	Homocysteine	61	-0.414	-0.620	23.479	0.430	135	6	134	7	118	61 original
2308	18 [590; 1-Acetyl-2-thiocydi]	82	Lysine	38	-0.460	-0.729	16.291	0.467	136	5	140	1	79	22 original
2251	18 [590; 1-Acetyl-2-thiocydi]	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.463	-0.580	17.500	0.475	137	4	132	8	92	17 original
10510	18 [590; 1-Acetyl-2-thiocydi]	5	Leucine	45	-0.485	-0.649	12.498	0.488	138	3	137	4	58	9 duplicate
2275	18 [590; 1-Acetyl-2-thiocydi]	49	[877; Pyrophosphoric acid (4TMS)]	64	-0.495	-0.664	23.081	0.458	139	2	138	3	116	35 original
2246	18 [590; 1-Acetyl-2-thiocydi]	20	[619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.553	-0.712	16.716	0.460	140	1	139	2	85	31 original
2389	19 Alanine (BP) (3TMS)	41	[639; Proline (2TMS)]	64	0.759	0.932	3.630	0.658	1	140	1	140	1	1 original
2462	19 Alanine (BP) (3TMS)	114	Fructose-6-phosphate	53	0.688	0.845	12.169	0.565	2	139	3	138	44	18 original
2471	19 Alanine (BP) (3TMS)	123	[945; Galactofuranose-6-phosphate (7TMS)]	64	0.623	0.850	3.748	0.603	3	138	2	139	2	5 original
2461	19 Alanine (BP) (3TMS)	113	Galactose-6-phosphate	62	0.599	0.830	11.978	0.568	4	137	4	137	41	18 original
2452	19 Alanine (BP) (3TMS)	104	[795; Erythritol (4TMS)]	63	0.564	0.717	8.693	0.581	5	136	18	123	18	12 original
2454	19 Alanine (BP) (3TMS)	106	[733; Threitol (4TMS)]	62	0.552	0.800	7.559	0.602	6	135	9	132	13	6 original
2421	19 Alanine (BP) (3TMS)	73	[708; Glucose methoxamine (5TMS)]	57	0.533	0.743	12.522	0.482	7	134	14	127	48	71 original
2463	19 Alanine (BP) (3TMS)	115	Glucose-6-phosphate	62	0.530	0.815	14.838	0.527	8	133	5	136	67	39 original
2374	19 Alanine (BP) (3TMS)	26	Citramalic acid	64	0.527	0.704	8.114	0.488	9	132	20	121	16	65 original
2383	19 Alanine (BP) (3TMS)	35	Pyroglutamic acid	64	0.501	0.809	31.879	0.546	10	131	7	134	138	30 original
2426	19 Alanine (BP) (3TMS)	78	Mannose	62	0.489	0.755	13.491	0.516	11	130	12	129	57	48 original
12188	19 Alanine (BP) (3TMS)	18	[590; 1-Acetyl-2-thiocydi]	64	0.478	0.677	6.486	0.462	12	129	23	118	6	87 duplicate
2469	19 Alanine (BP) (3TMS)	121	[657; Erythritol (4TMS)]	55	0.475	0.727	18.917	0.514	13	128	15	126	93	49 original
2418	19 Alanine (BP) (3TMS)	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	0.472	0.651	9.787	0.489	14	127	29	112	27	63 original
2424	19 Alanine (BP) (3TMS)	76	Fructose	64	0.469	0.814	15.482	0.546	15	126	6	135	75	31 original
2388	19 Alanine (BP) (3TMS)	40	[880; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.461	0.673	25.505	0.489	16	125	24	117	130	64 original
10646	19 Alanine (BP) (3TMS)	6	Glycerol	64	0.454	0.707	32.535	0.538	17	124	19	122	139	37 duplicate
2473	19 Alanine (BP) (3TMS)	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	0.450	0.803	21.874	0.524	18	123	8	133	105	40 original
2376	19 Alanine (BP) (3TMS)	28	Malic acid	64	0.441	0.649	5.447	0.494	19	122	30	111	3	61 original
2369	19 Alanine (BP) (3TMS)	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	0.438	0.633	7.871	0.455	20	121	34	107	14	91 original
2427	19 Alanine (BP) (3TMS)	79	Glucose	64	0.437	0.744	25.218	0.558	21	120	13	128	126	24 original
2465	19 Alanine (BP) (3TMS)	117	[724; Glycerol (3TMS)]	56	0.432	0.684	11.249	0.521	22	119	22	119	36	44 original
11690	19 Alanine (BP) (3TMS)	14	Fumaric acid	64	0.430	0.661	14.596	0.462	23	118	26	115	65	88 duplicate
2464	19 Alanine (BP) (3TMS)	116	[882; Pseudouridine (5TMS)]	30	0.425	0.223	12.374	0.339	24	117	73	68	47	136 original
2428	19 Alanine (BP) (3TMS)	80	[772; D-Glucose (5TMS)]	62	0.405	0.718	21.016	0.494	25	116	17	124	101	60 original
2435	19 Alanine (BP) (3TMS)	87	[945; beta-D-Glucopyranose (5TMS)]	62	0.398	0.769	25.351	0.523	26	115	10	131	128	42 original
11816	19 Alanine (BP) (3TMS)	15	Alanine	64	0.398	0.644	9.295	0.509	27	114	31	110	23	50 duplicate
2370	19 Alanine (BP) (3TMS)	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.394	0.579	17.212	0.469	28	113	44	97	85	83 original
2410	19 Alanine (BP) (3TMS)	62	[812; D-Xylofuranose (4TMS)]	64	0.393	0.681	5.884	0.519	29	112	21	120	4	45 original
2458	19 Alanine (BP) (3TMS)	110	[715; Erythritol (4TMS)]	54	0.391	0.722	16.100	0.612	30	111	16	125	70	3 original
2431	19 Alanine (BP) (3TMS)	83	Sorbitol	58	0.377	0.161	13.910	0.372	31	110	77	64	60	130 original
2434	19 Alanine (BP) (3TMS)	86	[783; D-Galactono-1,4-lactone (4TMS)]	61	0.375	0.758	15.176	0.558	32	109	11	130	71	25 original

11306	19 Alanine (BP) (3TMS)	11 Succinic acid	64 0.370	0.616	6.636	0.448	33	108	35	106	7	99 duplicate
2480	19 Alanine (BP) (3TMS)	132 [895; Isomaltose methoxyamine (8TMS)]	42 0.368	0.503	19.970	0.441	34	107	55	88	94	105 original
2422	19 Alanine (BP) (3TMS)	74 [912; Tetradecanoic acid (1TMS)]	64 0.360	0.641	12.192	0.496	35	106	32	109	45	59 original
2470	19 Alanine (BP) (3TMS)	122 [844; Erythritol (4TMS)]	52 0.356	0.603	20.986	0.564	36	105	36	105	100	19 original
2412	19 Alanine (BP) (3TMS)	64 [789; Tyramine (3TMS)]	63 0.337	0.459	10.584	0.397	37	104	59	82	31	120 original
2386	19 Alanine (BP) (3TMS)	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	64 0.325	0.587	7.088	0.458	38	103	40	101	11	90 original
2433	19 Alanine (BP) (3TMS)	85 [529; Methylethylsuccinic acid (4TMS)]	48 0.323	0.524	8.950	0.453	39	102	51	90	19	93 original
2436	19 Alanine (BP) (3TMS)	88 Gluconic acid	64 0.319	0.585	8.010	0.579	40	101	41	100	15	13 original
11563	19 Alanine (BP) (3TMS)	13 Uracil	64 0.313	0.583	8.532	0.544	41	100	42	99	17	32 duplicate
2486	19 Alanine (BP) (3TMS)	138 [674; Ergosterol (1TMS)]	46 0.306	0.477	20.632	0.473	42	99	58	83	98	79 original
2387	19 Alanine (BP) (3TMS)	39 [829; 1-Phenylethanol (1TMS)]	63 0.303	0.572	10.736	0.482	43	98	45	96	34	69 original
2481	19 Alanine (BP) (3TMS)	133 [855; Squalene]	64 0.302	0.361	9.603	0.436	44	97	65	76	25	108 original
2466	19 Alanine (BP) (3TMS)	118 [928; Glucopyranose-6-phosphate (6TMS)]	58 0.299	0.554	12.784	0.434	45	96	48	93	50	110 original
2460	19 Alanine (BP) (3TMS)	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63 0.292	0.510	22.757	0.498	46	95	53	88	111	55 original
2448	19 Alanine (BP) (3TMS)	100 [857; Mannitol (6TMS)]	64 0.292	0.360	6.813	0.431	47	94	66	75	9	112 original
2404	19 Alanine (BP) (3TMS)	56 [828; Orolic acid (3TMS)]	64 0.280	0.657	14.005	0.559	48	93	27	114	63	23 original
2392	19 Alanine (BP) (3TMS)	44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	50 0.277	0.489	10.696	0.524	49	92	56	85	32	41 original
11941	19 Alanine (BP) (3TMS)	24 [725; 2-Ketocanoic acid (2TMS)]	64 0.275	0.598	22.756	0.558	50	90	38	103	110	26 original
2474	19 Alanine (BP) (3TMS)	16 [844; 2-Methyl-1,3-butanediol (2TMS)]	45 0.273	0.547	9.292	0.544	51	91	50	91	22	33 duplicate
2450	19 Alanine (BP) (3TMS)	128 [536; Erythritol (4TMS)]	64 0.270	0.354	12.120	0.424	53	88	67	74	43	114 original
2444	19 Alanine (BP) (3TMS)	102 [904; Galactose methoxyamine (5TMS)]	49 0.269	0.263	24.449	0.304	54	87	71	70	119	140 original
2394	19 Alanine (BP) (3TMS)	96 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17 0.265	0.385	7.061	0.319	55	86	63	78	10	139 original
12065	19 Alanine (BP) (3TMS)	46 Arabinose	64 0.258	0.672	12.058	0.557	56	85	25	116	42	27 original
2377	19 Alanine (BP) (3TMS)	17 [700; 2-methyl-1,2-propanediol (2TMS)]	64 0.254	0.551	9.358	0.480	57	83	49	92	24	74 duplicate
2398	19 Alanine (BP) (3TMS)	29 Erythritol	64 0.254	0.507	10.070	0.470	58	84	54	87	28	82 original
2482	19 Alanine (BP) (3TMS)	50 [746; Ribonic acid-1,4-lactone (3TMS)]	61 0.247	0.520	24.729	0.467	59	82	52	89	122	86 original
2413	19 Alanine (BP) (3TMS)	134 Isomaltose	64 0.243	0.652	16.368	0.560	60	81	28	113	80	21 original
2468	19 Alanine (BP) (3TMS)	65 [846; 3-Deoxyglucitol (5TMS)]	63 0.228	0.641	15.461	0.569	61	80	33	108	74	15 original
		120 [945; Uridine (3TMS)]	54 0.226	0.137	7.302	0.468	62	79	79	62	12	85 original
2483	19 Alanine (BP) (3TMS)	135 [902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64 0.221	0.400	6.246	0.469	63	78	62	79	5	84 original
2451	19 Alanine (BP) (3TMS)	103 [848; Ethylamine (2TMS)]	63 0.215	0.366	13.175	0.492	64	77	64	77	54	82 original
11435	19 Alanine (BP) (3TMS)	12 Glycemic acid	63 0.208	0.450	17.057	0.441	65	76	60	81	83	104 duplicate
2457	19 Alanine (BP) (3TMS)	109 Octadecanoic acid	64 0.208	0.571	13.987	0.497	66	75	46	95	62	57 original
2488	19 Alanine (BP) (3TMS)	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49 0.194	0.203	20.836	0.455	67	74	74	67	99	92 original
2459	19 Alanine (BP) (3TMS)	111 [583; Erythritol (4TMS)]	42 0.192	0.312	25.904	0.472	68	73	69	72	131	81 original
2477	19 Alanine (BP) (3TMS)	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	59 0.190	0.587	12.651	0.581	69	72	39	102	49	11 original
2449	19 Alanine (BP) (3TMS)	101 [832; Dopamine (4TMS)]	64 0.184	0.275	11.753	0.452	70	71	70	71	40	96 original
2406	19 Alanine (BP) (3TMS)	58 [636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64 0.174	0.135	10.166	0.380	71	70	80	61	29	129 original
2442	19 Alanine (BP) (3TMS)	94 Hexadecanoic acid	64 0.166	0.478	12.986	0.544	72	69	57	84	53	34 original
2402	19 Alanine (BP) (3TMS)	54 [NA]	55 0.142	0.432	17.671	0.507	73	68	61	80	88	52 original
2475	19 Alanine (BP) (3TMS)	127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	39 0.131	0.230	9.690	0.426	74	67	72	69	28	113 original
2478	19 Alanine (BP) (3TMS)	130 Trehalose	63 0.110	0.055	21.324	0.369	75	66	83	58	103	131 original
2439	19 Alanine (BP) (3TMS)	91 [766; beta-D-Methylglucopyranoside (4TMS)]	64 0.098	0.175	17.528	0.481	76	65	75	66	86	72 original
2394	19 Alanine (BP) (3TMS)	36 [596; N-Acetylglutamic acid (2TMS)]	64 0.096	0.017	20.532	0.413	77	64	86	55	97	118 original
2419	19 Alanine (BP) (3TMS)	71 [731; Erythrose (3TMS)]	64 0.088	0.130	6.732	0.475	78	63	81	60	8	77 original
2440	19 Alanine (BP) (3TMS)	92 [680; Glycerol-2-phosphate (4TMS)]	54 0.082	0.600	11.433	0.523	79	62	37	104	37	43 original
2423	19 Alanine (BP) (3TMS)	75 Lysine	64 0.081	0.058	31.027	0.386	80	61	82	59	137	127 original

2405	19 Alanine (BP) (3TMS)	57	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55	0.067	0.554	12.285	0.531	81	59	47	94	48	38 original
2489	19 Alanine (BP) (3TMS)	141	Lanosta-8,24-dien-3-beta-ol	61	0.067	0.048	20.076	0.474	82	60	84	57	96	78 original
2487	19 Alanine (BP) (3TMS)	139	[700; Ergosta-5,7-dien-3-ol]	38	0.053	-0.013	22.897	0.437	83	58	89	52	112	107 original
2485	19 Alanine (BP) (3TMS)	137	Ergosterol	64	0.053	0.043	11.091	0.400	84	57	85	56	35	119 original
10375	19 Alanine (BP) (3TMS)	4	Phosphoric acid	51	0.023	-0.022	25.365	0.334	85	56	90	51	129	137 duplicate
2420	19 Alanine (BP) (3TMS)	72	[919; D-Xylopyranose (4TMS)]	63	-0.006	-0.003	14.614	0.355	86	55	87	54	68	135 original
2476	19 Alanine (BP) (3TMS)	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	-0.006	0.153	9.246	0.518	87	54	78	63	21	48 original
2408	19 Alanine (BP) (3TMS)	60	Glycerol-3-phosphate	64	-0.030	-0.152	13.931	0.607	88	53	96	45	61	4 original
2472	19 Alanine (BP) (3TMS)	124	[734; 1-Monocleoylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	59	-0.049	-0.138	29.746	0.381	89	52	94	47	136	128 original
10780	19 Alanine (BP) (3TMS)	7	Threonine	64	-0.051	-0.049	21.730	0.396	90	51	91	50	104	121 duplicate
2447	19 Alanine (BP) (3TMS)	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	-0.071	0.325	15.458	0.499	91	50	68	73	73	54 original
2395	19 Alanine (BP) (3TMS)	47	[NA]	64	-0.073	-0.013	13.900	0.449	92	49	88	53	59	88 original
2414	19 Alanine (BP) (3TMS)	66	Glycic acid-3-phosphate	64	-0.083	-0.118	12.813	0.450	93	48	93	48	51	97 original
2445	19 Alanine (BP) (3TMS)	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	-0.090	0.168	16.162	0.559	94	47	76	65	78	22 original
10100	19 Alanine (BP) (3TMS)	2	Serine	62	-0.127	-0.117	16.232	0.364	95	46	92	49	79	133 duplicate
2438	19 Alanine (BP) (3TMS)	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	64	-0.149	-0.310	10.367	0.473	96	45	106	35	30	80 original
2455	19 Alanine (BP) (3TMS)	107	9-(Z)-Octadecenoic acid	64	-0.151	-0.303	9.192	0.477	97	44	105	36	20	76 original
2432	19 Alanine (BP) (3TMS)	84	Mannitol	62	-0.156	-0.159	24.927	0.444	98	43	97	44	124	102 original
2453	19 Alanine (BP) (3TMS)	105	[705; 2-Ketogluconic acid (5TMS)]	48	-0.158	-0.204	13.202	0.543	99	42	99	42	55	36 original
2415	19 Alanine (BP) (3TMS)	67	Citric acid	64	-0.161	-0.277	15.751	0.517	100	41	104	37	77	47 original
2467	19 Alanine (BP) (3TMS)	119	[931; myo-Inositol-2-phosphate (7TMS)]	64	-0.169	-0.276	11.478	0.481	101	40	103	38	38	73 original
2446	19 Alanine (BP) (3TMS)	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	48	-0.186	-0.429	23.777	0.446	102	39	118	23	116	100 original
2456	19 Alanine (BP) (3TMS)	108	Octadecenoic acid	64	-0.197	-0.258	13.882	0.395	103	38	101	40	58	123 original
2385	19 Alanine (BP) (3TMS)	37	Phenylalanine	64	-0.207	-0.268	14.977	0.483	104	37	102	39	69	68 original
2375	19 Alanine (BP) (3TMS)	63	-0.216	53	-0.218	-0.318	22.026	0.501	105	36	109	32	106	53 original
2401	19 Alanine (BP) (3TMS)	32	[729; N,N-Dimethyllysine methyl ester]	53	-0.218	-0.505	24.748	0.432	106	35	121	20	123	111 original
11045	19 Alanine (BP) (3TMS)	53	Glycerol-2-phosphate	64	-0.236	-0.363	17.753	0.445	107	34	113	28	88	101 original
2379	19 Alanine (BP) (3TMS)	9	Proline	63	-0.247	-0.169	22.444	0.365	108	33	98	43	108	132 duplicate
2391	19 Alanine (BP) (3TMS)	31	[622; Parabanic acid (2TMS)]	64	-0.248	-0.378	17.663	0.424	109	32	115	26	87	115 original
2429	19 Alanine (BP) (3TMS)	43	[548; Leucine (2TBS)]	60	-0.258	-0.380	10.715	0.442	110	31	116	25	33	103 original
2407	19 Alanine (BP) (3TMS)	81	Tyrosine	64	-0.277	-0.474	27.356	0.585	111	30	120	21	132	10 original
10238	19 Alanine (BP) (3TMS)	59	Ornithine; Arginine	64	-0.288	-0.310	32.715	0.396	112	29	107	34	140	122 original
9961	19 Alanine (BP) (3TMS)	3	Ethanolamine	36	-0.321	-0.552	18.297	0.561	113	28	124	17	92	20 duplicate
2373	19 Alanine (BP) (3TMS)	1	[938; Sulfuric acid (2TMS)]	36	-0.321	-0.226	13.246	0.497	114	27	100	41	56	56 duplicate
2441	19 Alanine (BP) (3TMS)	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.324	-0.442	21.043	0.497	115	26	119	22	102	58 original
2371	19 Alanine (BP) (3TMS)	93	[607; Putrescine (4TMS)]	60	-0.331	-0.320	23.480	0.436	116	25	110	31	115	109 original
2425	19 Alanine (BP) (3TMS)	23	Homoserine	64	-0.334	-0.566	14.945	0.459	117	24	125	16	68	89 original
2382	19 Alanine (BP) (3TMS)	77	[826; beta-[(5-methyl-2-thienyl)methylenamino-benzeneacetic acid methyl ester]	62	-0.341	-0.388	24.163	0.395	118	23	117	24	117	124 original
2381	19 Alanine (BP) (3TMS)	34	Aspartic acid	64	-0.368	-0.361	25.293	0.394	119	22	112	29	127	126 original
10913	19 Alanine (BP) (3TMS)	33	Methionine	64	-0.373	-0.376	14.393	0.413	120	21	114	27	64	117 original
11776	19 Alanine (BP) (3TMS)	8	Isoleucine	55	-0.375	-0.145	15.667	0.322	121	20	95	46	78	138 duplicate
2390	19 Alanine (BP) (3TMS)	30	[815; Ethyl-3(2H)-thiophenone]	64	-0.387	-0.313	23.276	0.363	122	19	108	33	114	134 original
2417	19 Alanine (BP) (3TMS)	10	Glycine	64	-0.397	-0.685	15.234	0.544	123	18	130	11	72	35 duplicate
2393	19 Alanine (BP) (3TMS)	42	Glutamic acid	60	-0.398	-0.337	24.945	0.394	124	17	111	30	125	125 original
2478	19 Alanine (BP) (3TMS)	69	Arginine	60	-0.398	-0.542	17.990	0.488	125	16	122	19	90	68 original
2409	19 Alanine (BP) (3TMS)	45	Homocysteine	61	-0.447	-0.573	28.083	0.422	126	15	126	15	135	118 original
		131	[826; 5-Methylthioadenosine (3TMS)]	55	-0.453	-0.781	23.020	0.597	127	14	132	9	113	7 original
		61	[NA]	64	-0.454	-0.640	11.660	0.482	128	13	127	14	39	70 original

2386	19 Alanine (BP) (3TMS)	48 Asparagine	64 -0.460	-0.764	17,118	0.566	129	12	131	10	84	17 original
2397	19 Alanine (BP) (3TMS)	49 [877; Pyrophosphoric acid (4TMS)]	64 -0.477	-0.677	27,906	0.441	130	11	129	12	134	106 original
2399	19 Alanine (BP) (3TMS)	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44 -0.486	-0.549	24,705	0.452	131	10	123	18	121	85 original
2368	19 Alanine (BP) (3TMS)	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31 -0.531	-0.915	20,054	0.619	132	9	140	1	95	2 original
2403	19 Alanine (BP) (3TMS)	[612; 4-Aminobutyric acid (2TBS)]	43 -0.568	-0.862	27,813	0.550	133	8	136	5	133	29 original
2443	19 Alanine (BP) (3TMS)	[55; 770; 3,4,6-Trishydroxyphenylethanolamine (5TMS)]	50 -0.610	-0.788	24,218	0.591	134	7	133	8	118	9 original
2400	19 Alanine (BP) (3TMS)	52 [NA]	46 -0.614	-0.860	24,686	0.573	135	6	135	6	120	14 original
2430	19 Alanine (BP) (3TMS)	82 Lysine	39 -0.628	-0.864	18,213	0.593	136	5	137	4	91	8 original
2411	19 Alanine (BP) (3TMS)	63 Glutamine	52 -0.643	-0.813	22,597	0.478	137	4	134	7	109	75 original
2416	19 Alanine (BP) (3TMS)	[68; 570; Hypoxanthine (2TMS)]	20 -0.674	-0.880	16,375	0.484	138	3	139	2	81	84 original
10511	19 Alanine (BP) (3TMS)	5 Leucine	45 -0.681	-0.661	16,672	0.452	139	2	128	13	82	94 duplicate
2437	19 Alanine (BP) (3TMS)	[89; 775; Dopamine (4TMS)]	35 -0.724	-0.877	22,235	0.508	140	1	138	3	107	51 original
2600	20 [619; 2-(3',4'-Bishydroxy	[131; 626; 5-Methylthioadenosine (3TMS)]	27 0.738	0.914	5,417	0.685	1	140	7	134	5	5 original
2511	20 [619; 2-(3',4'-Bishydroxy	42 Glutamic acid	31 0.690	0.654	34,981	0.599	2	139	22	119	133	52 original
11177	20 [619; 2-(3',4'-Bishydroxy	10 Glycine	31 0.800	0.907	25,647	0.672	3	138	8	133	110	13 duplicate
2576	20 [619; 2-(3',4'-Bishydroxy	107 9-(Z)-Octadecenoic acid	31 0.578	0.591	20,771	0.445	4	137	27	114	98	118 original
2517	20 [619; 2-(3',4'-Bishydroxy	48 Asparagine	31 0.561	0.880	17,273	0.676	5	136	11	130	83	10 original
2494	20 [619; 2-(3',4'-Bishydroxy	25 [709; 2,5-Diaminovalerolactam (2TMS)]	17 0.559	0.785	14,728	0.530	6	135	14	127	56	92 original
2522	20 [619; 2-(3',4'-Bishydroxy	53 Glycerol-2-phosphate	31 0.553	0.669	8,841	0.465	7	134	20	121	14	111 original
2559	20 [619; 2-(3',4'-Bishydroxy	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	31 0.544	0.552	14,531	0.549	8	133	32	109	54	81 original
2518	20 [619; 2-(3',4'-Bishydroxy	49 [877; Pyrophosphoric acid (4TMS)]	31 0.535	0.760	6,953	0.513	9	132	15	128	8	100 original
10239	20 [619; 2-(3',4'-Bishydroxy	3 Ethanolamine	30 0.531	0.898	10,661	0.683	10	131	9	132	25	6 duplicate
2562	20 [619; 2-(3',4'-Bishydroxy	93 [607; Putrescine (4TMS)]	29 0.522	0.721	7,012	0.529	11	130	18	123	9	93 original
2550	20 [619; 2-(3',4'-Bishydroxy	81 Tyrosine	31 0.501	0.920	37,926	0.697	12	129	6	135	137	3 original
2551	20 [619; 2-(3',4'-Bishydroxy	82 Lysine	26 0.489	0.956	20,677	0.682	13	128	3	138	97	7 original
2546	20 [619; 2-(3',4'-Bishydroxy	[77; 826; beta-[[[5-methyl-2-thienyl)methyleneamino- benzeneacetic acid methyl ester]	31 0.480	0.873	35,085	0.643	14	127	13	128	134	30 original
2524	20 [619; 2-(3',4'-Bishydroxy	55 [612; 4-Aminobutyric acid (2TBS)]	29 0.463	0.924	4,165	0.681	15	126	5	136	2	19 original
10512	20 [619; 2-(3',4'-Bishydroxy	5 Leucine	29 0.453	0.722	10,569	0.573	16	125	17	124	24	68 duplicate
2499	20 [619; 2-(3',4'-Bishydroxy	30 [815; Ethyl-3(2H)-thiophenone]	31 0.445	0.625	33,834	0.581	17	124	25	116	129	60 original
2588	20 [619; 2-(3',4'-Bishydroxy	119 [931; myo-Inositol-2-phosphate (7TMS)]	31 0.441	0.556	14,956	0.606	18	123	30	111	58	47 original
2577	20 [619; 2-(3',4'-Bishydroxy	108 Octadecanoic acid	31 0.424	0.496	12,987	0.428	19	122	38	103	38	124 original
2564	20 [619; 2-(3',4'-Bishydroxy	95 [770; 3,4,6-Trishydroxyphenylethanolamine (5TMS)]	26 0.422	0.894	3,906	0.702	20	121	10	131	1	2 original
2530	20 [619; 2-(3',4'-Bishydroxy	61 [NA]	31 0.402	0.537	14,141	0.513	21	120	36	105	50	101 original
2553	20 [619; 2-(3',4'-Bishydroxy	84 Mannitol	31 0.389	0.608	27,478	0.487	22	119	28	115	117	107 original
2520	20 [619; 2-(3',4'-Bishydroxy	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	28 0.386	0.647	6,611	0.608	23	118	23	118	7	46 original
2521	20 [619; 2-(3',4'-Bishydroxy	52 [NA]	23 0.368	0.938	4,537	0.693	24	117	4	137	3	4 original
2528	20 [619; 2-(3',4'-Bishydroxy	59 Ornithine; Arginine	31 0.355	0.714	40,806	0.599	25	118	19	122	140	50 original
2558	20 [619; 2-(3',4'-Bishydroxy	89 [775; Dopamine (4TMS)]	23 0.344	0.965	7,496	0.664	26	115	1	140	10	16 original
2502	20 [619; 2-(3',4'-Bishydroxy	33 Methionine	31 0.329	0.582	17,267	0.617	27	114	28	113	82	41 original
2538	20 [619; 2-(3',4'-Bishydroxy	69 Arginine	31 0.303	0.730	27,967	0.654	28	112	16	125	120	24 original
2503	20 [619; 2-(3',4'-Bishydroxy	34 Aspartic acid	31 0.303	0.538	34,800	0.594	29	113	35	106	132	55 original
2514	20 [619; 2-(3',4'-Bishydroxy	45 Homocysteine	31 0.295	0.551	7,923	0.504	30	111	33	108	11	102 original
2593	20 [619; 2-(3',4'-Bishydroxy	[124; 734; 1-Monooleoylglycerol (2TMS); 1- Monohexadecanoylglycerol (1TMS)]	28 0.280	0.304	9,398	0.429	31	110	42	99	17	122 original
2563	20 [619; 2-(3',4'-Bishydroxy	94 Hexadecanoic acid	31 0.260	-0.369	26,007	0.613	32	109	63	78	112	44 original
2536	20 [619; 2-(3',4'-Bishydroxy	67 Citric acid	31 0.252	0.554	27,804	0.599	33	108	31	110	119	51 original
2599	20 [619; 2-(3',4'-Bishydroxy	130 Trehalose	30 0.241	0.225	31,419	0.340	34	107	46	95	124	133 original
2532	20 [619; 2-(3',4'-Bishydroxy	63 Glutamine	24 0.239	0.876	11,739	0.641	35	106	12	129	32	31 original
10914	20 [619; 2-(3',4'-Bishydroxy	8 Isoleucine	31 0.230	0.548	24,308	0.466	36	105	34	107	107	110 duplicate

2610	20 [619; 2-(3',4'-Bishydroxy	141	Lanosta-8,24-dien-3-beta-ol	31	0.217	0.217	9.804	0.527	37	104	47	94	18	95 original
2606	20 [619; 2-(3',4'-Bishydroxy	137	Ergosterol	31	0.209	0.254	20.335	0.530	38	103	44	97	95	91 original
2506	20 [619; 2-(3',4'-Bishydroxy	37	Phenylalanine	31	0.204	0.465	27.528	0.577	39	102	40	101	118	-63 original
2578	20 [619; 2-(3',4'-Bishydroxy	109	Octadecanoic acid	31	0.196	-0.547	25.994	0.598	40	101	70	71	111	53 original
2501	20 [619; 2-(3',4'-Bishydroxy	32	[729; N,N-Dimethyllysine methyl ester]	31	0.187	0.629	13.922	0.668	41	100	24	117	47	14 original
11046	20 [619; 2-(3',4'-Bishydroxy	9	Proline	31	0.183	0.531	32.218	0.582	42	99	37	104	125	59 duplicate
2500	20 [619; 2-(3',4'-Bishydroxy	31	[622; Parabenic acid (2TMS)]	31	0.178	0.487	11.268	0.551	43	98	39	102	28	79 original
2529	20 [619; 2-(3',4'-Bishydroxy	60	Glycerol-3-phosphate	31	0.166	0.328	27.002	0.581	44	97	41	100	116	61 original
2492	20 [619; 2-(3',4'-Bishydroxy	23	Homoserine	31	0.131	0.654	17.050	0.662	45	96	21	120	81	18 original
2537	20 [619; 2-(3',4'-Bishydroxy	68	[570; Hypoxanthine (2TMS)]	14	0.077	0.957	5.332	0.615	46	95	2	139	4	42 original
2541	20 [619; 2-(3',4'-Bishydroxy	72	[919; D-Xylopyranose (4TMS)]	31	0.062	0.108	13.302	0.265	47	94	50	91	43	138 original
2609	20 [619; 2-(3',4'-Bishydroxy	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	25	0.040	-0.076	9.170	0.545	48	93	56	85	15	85 original
2608	20 [619; 2-(3',4'-Bishydroxy	139	[700; Ergosta-5,7-dien-3-ol]	18	0.020	0.063	8.714	0.476	49	92	51	90	13	108 original
2543	20 [619; 2-(3',4'-Bishydroxy	74	[912; Tetradecanoic acid (1TMS)]	31	0.019	-0.579	15.862	0.614	50	91	73	68	72	43 original
10781	20 [619; 2-(3',4'-Bishydroxy	7	Threonine	31	-0.015	-0.008	32.535	0.573	51	90	55	86	128	69 duplicate
2516	20 [619; 2-(3',4'-Bishydroxy	47	[NA]	31	-0.019	0.012	14.532	0.329	52	89	54	87	55	137 original
2544	20 [619; 2-(3',4'-Bishydroxy	75	Lysine	31	-0.024	-0.142	39.655	0.528	53	88	58	83	139	94 original
2512	20 [619; 2-(3',4'-Bishydroxy	43	[548; Leucine (2TBS)]	31	-0.037	0.242	16.090	0.618	54	86	45	96	74	40 original
2505	20 [619; 2-(3',4'-Bishydroxy	36	[596; N-Acetylglutamic acid (2TMS)]	31	-0.037	0.020	32.423	0.526	55	87	52	89	127	96 original
10376	20 [619; 2-(3',4'-Bishydroxy	4	Phosphoric acid	30	-0.062	-0.086	36.549	0.364	56	85	57	84	135	131 duplicate
10101	20 [619; 2-(3',4'-Bishydroxy	2	Serine	31	-0.097	0.136	25.031	0.585	57	82	48	93	109	57 duplicate
2535	20 [619; 2-(3',4'-Bishydroxy	66	Glyceric acid-3-phosphate	31	-0.097	0.108	13.415	0.544	58	83	49	92	45	86 original
2554	20 [619; 2-(3',4'-Bishydroxy	85	[528; Methylcitic acid (4TMS)]	31	-0.097	-0.515	14.118	0.504	59	84	69	72	49	103 original
2585	20 [619; 2-(3',4'-Bishydroxy	116	[882; Pseudouridine (5TMS)]	18	-0.124	0.017	11.482	0.429	60	81	53	88	31	123 original
[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane														
2527	20 [619; 2-(3',4'-Bishydroxy	58	[674; Ergosterol (1TMS)]	31	-0.127	-0.322	23.030	0.518	61	80	61	80	105	99 original
2607	20 [619; 2-(3',4'-Bishydroxy	138	[674; Ergosterol (1TMS)]	20	-0.147	-0.641	10.203	0.588	62	79	77	64	22	56 original
2540	20 [619; 2-(3',4'-Bishydroxy	71	[731; Erythrose (3TMS)]	31	-0.170	-0.213	19.698	0.560	63	77	59	82	91	75 original
2602	20 [619; 2-(3',4'-Bishydroxy	133	[855; Squalene]	31	-0.170	-0.365	15.894	0.441	64	78	62	79	73	120 original
2568	20 [619; 2-(3',4'-Bishydroxy	99	[662; Ribose-5-phosphate methoxamine (BP) (5TMS)]	14	-0.187	-0.676	10.027	0.434	65	76	78	63	21	121 original
135														
2604	20 [619; 2-(3',4'-Bishydroxy	902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	31	-0.191	-0.423	19.205	0.548	66	75	68	75	89	83 original	
2587	20 [619; 2-(3',4'-Bishydroxy	98	[897; Ribose-5-phosphate methoxamine (5TMS)]	23	-0.202	0.293	6.298	0.640	67	74	43	98	6	33 original
2496	20 [619; 2-(3',4'-Bishydroxy	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	30	-0.214	0.567	9.852	0.649	68	73	28	112	19	26 original
2589	20 [619; 2-(3',4'-Bishydroxy	100	[857; Mannitol (6TMS)]	31	-0.247	-0.429	16.292	0.464	69	72	67	74	75	114 original
2571	20 [619; 2-(3',4'-Bishydroxy	102	[904; Galactose methoxamine (5TMS)]	31	-0.273	-0.436	12.877	0.456	70	71	68	73	37	117 original
2581	20 [619; 2-(3',4'-Bishydroxy	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	30	-0.278	-0.557	9.905	0.568	71	70	71	70	20	73 original
11436	20 [619; 2-(3',4'-Bishydroxy	12	Glyceric acid	30	-0.301	-0.605	11.112	0.548	72	69	74	67	27	82 duplicate
2568	20 [619; 2-(3',4'-Bishydroxy	97	[756; beta-D-Methylglucopyranoside (4TMS)]	19	-0.310	-0.806	18.532	0.444	73	68	97	44	87	119 original
2565	20 [619; 2-(3',4'-Bishydroxy	96	myo-Inositol	26	-0.323	-0.232	10.443	0.340	74	67	60	81	23	134 original
2587	20 [619; 2-(3',4'-Bishydroxy	118	[928; Glucopyranose-6-phosphate (6TMS)]	25	-0.333	-0.577	14.991	0.378	75	66	72	69	60	129 original
2560	20 [619; 2-(3',4'-Bishydroxy	91	[766; beta-D-Methylglucopyranoside (4TMS)]	31	-0.359	-0.628	14.844	0.625	76	65	76	65	57	36 original
2589	20 [619; 2-(3',4'-Bishydroxy	120	[945; Uridine (3TMS)]	23	-0.368	-0.374	18.427	0.536	77	64	64	77	86	88 original
2548	20 [619; 2-(3',4'-Bishydroxy	79	Glucose	31	-0.381	-0.844	34.141	0.597	78	63	106	35	131	54 original
2580	20 [619; 2-(3',4'-Bishydroxy	111	[563; Erythritol (4TMS)]	16	-0.400	-0.394	8.074	0.386	79	62	65	76	12	127 original
2495	20 [619; 2-(3',4'-Bishydroxy	26	Citramalic acid	31	-0.415	-0.687	21.824	0.543	80	60	79	62	101	87 original
11817	20 [619; 2-(3',4'-Bishydroxy	15	Alanine	31	-0.415	-0.805	24.683	0.640	81	61	98	45	108	32 duplicate
2509	20 [619; 2-(3',4'-Bishydroxy	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	31	-0.419	-0.746	33.853	0.626	82	59	85	56	130	35 original
11691	20 [619; 2-(3',4'-Bishydroxy	14	Fumaric acid	31	-0.424	-0.767	11.951	0.621	83	58	87	54	34	38 duplicate
2573	20 [619; 2-(3',4'-Bishydroxy	104	[795; Erythritol (4TMS)]	31	-0.428	-0.861	15.818	0.624	84	57	109	32	70	37 original
2597	20 [619; 2-(3',4'-Bishydroxy	128	[924; D-Sedoheptulose-7-phosphate (7TMS)]	15	-0.429	-0.820	14.476	0.335	85	56	100	41	53	135 original



2549	20 [619; 2-(3',4'-Bishydroxy	80 [772; D-Glucose (5TMS)]	31 -0.445	-0.733	30.076	0.406	86	55	83	58	122	128 original
2553	20 [619; 2-(3',4'-Bishydroxy	64 [789; Tyramine (3TMS)]	30 -0.448	-0.614	14.049	0.380	87	54	75	66	48	128 original
2556	20 [619; 2-(3',4'-Bishydroxy	87 [945; beta-D-Glucopyranose (5TMS)]	31 -0.454	-0.768	32.357	0.370	88	53	92	49	126	130 original
2487	20 [619; 2-(3',4'-Bishydroxy	28 Malic acid	31 -0.458	-0.769	16.854	0.675	89	52	88	53	79	11 original
2491	20 [619; 2-(3',4'-Bishydroxy	22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	24 -0.464	-0.725	11.351	0.464	90	51	82	59	30	113 original
2596	20 [619; 2-(3',4'-Bishydroxy	127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	10 -0.467	-0.889	11.947	0.343	91	50	114	27	33	132 original
2570	20 [619; 2-(3',4'-Bishydroxy	101 [832; Dopamine (4TMS)]	31 -0.471	-0.701	13.748	0.651	92	48	80	61	48	25 original
11564	20 [619; 2-(3',4'-Bishydroxy	13 Uracil	31 -0.471	-0.892	19.262	0.656	93	49	116	25	90	22 duplicate
2574	20 [619; 2-(3',4'-Bishydroxy	105 [705; 2-Ketogluconic acid (5TMS)]	15 -0.486	-0.759	12.348	0.498	94	47	88	55	35	104 original
2510	20 [619; 2-(3',4'-Bishydroxy	41 [639; Proline (2TMS)]	31 -0.488	-0.803	21.098	0.532	95	46	94	47	100	90 original
2490	20 [619; 2-(3',4'-Bishydroxy	21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	31 -0.497	-0.744	21.911	0.574	96	45	84	57	102	66 original
12311	20 [619; 2-(3',4'-Bishydroxy	19 Alanine (BP) (3TMS)	31 -0.531	-0.915	20.054	0.619	97	44	128	15	94	39 duplicate
10647	20 [619; 2-(3',4'-Bishydroxy	6 Glyceral	31 -0.548	-0.861	38.465	0.520	98	43	108	33	138	98 duplicate
12189	20 [619; 2-(3',4'-Bishydroxy	18 [590; 1-Acetyl-2-thiohydantoin]	31 -0.553	-0.712	16.716	0.460	99	42	81	60	77	116 duplicate
2519	20 [619; 2-(3',4'-Bishydroxy	50 [746; Ribonic acid-1,4-lactone (3TMS)]	28 -0.556	-0.780	11.318	0.523	100	41	93	48	29	97 original
2498	20 [619; 2-(3',4'-Bishydroxy	29 Erythritol	31 -0.557	-0.771	13.320	0.546	101	40	90	51	44	84 original
2601	20 [619; 2-(3',4'-Bishydroxy	132 [895; Isomaltose methoxyamine (6TMS)]	14 -0.560	-0.832	13.222	0.424	102	39	103	38	42	125 original
11307	20 [619; 2-(3',4'-Bishydroxy	11 Succinic acid	31 -0.561	-0.813	15.855	0.549	103	38	98	43	71	80 duplicate
2575	20 [619; 2-(3',4'-Bishydroxy	106 [733; Threitol (4TMS)]	29 -0.567	-0.911	16.976	0.711	104	37	123	18	80	1 original
9862	20 [619; 2-(3',4'-Bishydroxy	1 [938; Sulfuric acid (2TMS)]	8 -0.571	-0.770	8.368	0.223	105	36	89	52	16	139 duplicate
2590	20 [619; 2-(3',4'-Bishydroxy	121 [657; Erythritol (4TMS)]	22 -0.576	-0.829	12.600	0.576	106	35	102	39	36	64 original
2508	20 [619; 2-(3',4'-Bishydroxy	39 [829; 1-Phenylethanol (1TMS)]	30 -0.588	-0.852	18.190	0.605	107	34	107	34	85	48 original
2592	20 [619; 2-(3',4'-Bishydroxy	123 [945; Galactofuranose-6-phosphate (7TMS)]	31 -0.591	-0.878	19.080	0.630	108	33	110	31	88	34 original
2572	20 [619; 2-(3',4'-Bishydroxy	103 [648; Ethylamine (2TMS)]	30 -0.595	-0.817	15.218	0.663	109	32	99	42	61	17 original
2539	20 [619; 2-(3',4'-Bishydroxy	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	30 -0.600	-0.895	22.995	0.461	110	30	117	24	103	115 original
2561	20 [619; 2-(3',4'-Bishydroxy	92 [680; Glycerol-2-phosphate (4TMS)]	21 -0.600	-0.902	15.707	0.330	111	31	118	23	68	136 original
2552	20 [619; 2-(3',4'-Bishydroxy	83 Sorbitol	31 -0.604	-0.782	26.917	0.571	112	28	91	50	115	106 original
2547	20 [619; 2-(3',4'-Bishydroxy	78 Mannose	30 -0.614	-0.886	15.531	0.571	113	28	113	28	65	72 original
2513	20 [619; 2-(3',4'-Bishydroxy	44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	17 -0.618	-0.841	15.628	0.470	114	27	104	37	67	109 original
2586	20 [619; 2-(3',4'-Bishydroxy	117 [724; Glycerol (3TMS)]	23 -0.621	-0.804	14.350	0.572	115	26	95	46	52	71 original
2598	20 [619; 2-(3',4'-Bishydroxy	128 [840; Maltose methoxyamine (6TMS); alpha-D-Glc-(1,4)-D-Glc]	26 -0.637	-0.910	14.961	0.604	116	25	120	21	59	49 original
2531	20 [619; 2-(3',4'-Bishydroxy	62 [812; D-Xylofuranose (4TMS)]	31 -0.639	-0.880	19.862	0.577	117	21	111	30	93	62 original
2542	20 [619; 2-(3',4'-Bishydroxy	73 [708; Glucose methoxyamine (5TMS)]	31 -0.639	-0.914	15.623	0.574	118	22	124	17	68	67 original
2525	20 [619; 2-(3',4'-Bishydroxy	56 [829; Oxalic acid (3TMS)]	31 -0.639	-0.960	15.442	0.668	119	23	136	5	63	15 original
2545	20 [619; 2-(3',4'-Bishydroxy	76 Fructose	24 -0.645	-0.972	26.267	0.655	120	24	140	1	113	23 original
2583	20 [619; 2-(3',4'-Bishydroxy	114 Fructose-6-phosphate	31 -0.647	-0.923	14.336	0.574	121	20	127	14	51	65 original
2603	20 [619; 2-(3',4'-Bishydroxy	54 [NA]	22 -0.654	-0.948	23.512	0.672	122	19	132	9	106	12 original
2523	20 [619; 2-(3',4'-Bishydroxy	88 Gluconic acid	31 -0.660	-0.911	13.052	0.464	123	18	122	19	40	112 original
2557	20 [619; 2-(3',4'-Bishydroxy	46 Arabinose	31 -0.660	-0.910	16.648	0.678	124	16	121	20	76	9 original
2515	20 [619; 2-(3',4'-Bishydroxy	126 [559; Erythritol (4TMS)]	31 -0.660	-0.963	19.732	0.644	125	17	137	4	92	29 original
2595	20 [619; 2-(3',4'-Bishydroxy	115 Glucose-6-phosphate	13 -0.667	-0.946	13.024	0.558	126	15	131	10	39	77 original
2584	20 [619; 2-(3',4'-Bishydroxy	86 [793; D-Galactono-1,4-lactone (4TMS)]	29 -0.670	-0.955	26.627	0.551	127	14	134	7	114	78 original
2555	20 [619; 2-(3',4'-Bishydroxy	65 [646; 3-Deoxyglucitol (5TMS)]	31 -0.677	-0.970	23.022	0.648	128	13	136	3	104	27 original
2534	20 [619; 2-(3',4'-Bishydroxy	122 [715; Erythritol (4TMS)]	30 -0.678	-0.941	16.845	0.647	129	12	129	12	78	28 original
2579	20 [619; 2-(3',4'-Bishydroxy	110 [644; Erythritol (4TMS)]	19 -0.686	-0.905	15.476	0.611	130	11	119	22	64	45 original
2591	20 [619; 2-(3',4'-Bishydroxy	113 Galactose-6-phosphate	29 -0.696	-0.826	13.171	0.535	131	10	101	40	41	89 original
2582	20 [619; 2-(3',4'-Bishydroxy	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	31 -0.712	-0.889	21.033	0.657	133	8	115	26	99	74 original
11942	20 [619; 2-(3',4'-Bishydroxy	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	31 -0.716	-0.843	15.230	0.573	134	7	105	38	62	70 original

2526	20 [619]: 2-(3',4'-Bishydroxy	[757]: 2-Desoxy-pentose-3-Yose dimethoxyamine (2TMS)]	22	-0.723	-0.955	17.475	0.494	135	6	135	6	84	105 original
12066	20 [619]: 2-(3',4'-Bishydroxy	[700]: 2-methyl-1,2-propanediol (2TMS)]	31	-0.729	-0.885	20.540	0.559	136	5	112	29	96	76 duplicate
2594	20 [619]: 2-(3',4'-Bishydroxy	[892]: Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	31	-0.738	-0.954	30.773	0.583	137	4	133	8	123	58 original
2493	20 [619]: 2-(3',4'-Bishydroxy	[725]: 2-Ketooctanoic acid (2TMS)]	31	-0.742	-0.933	29.683	0.681	138	3	128	13	121	8 original
2504	20 [619]: 2-(3',4'-Bishydroxy	35 Pyroglyutamic acid	31	-0.755	-0.971	37.648	0.657	139	2	139	2	136	20 original
2605	20 [619]: 2-(3',4'-Bishydroxy	[748]: D-Sedoheptulose-7-phosphate (7TMS)]	5	-1.000	-0.914	10.881	-0.002	140	1	125	16	28	140 original
12190	21 [678]: N,N-Di-(2-Hydroxy	[590]: 1-Acetyl-2-thiobutanolin]	64	0.726	0.883	10.588	0.550	1	140	1	140	26	25 duplicate
2617	21 [678]: N,N-Di-(2-Hydroxy	28 Malic acid	64	0.666	0.851	8.469	0.579	2	139	3	138	15	6 original
11692	21 [678]: N,N-Di-(2-Hydroxy	11 Fumaric acid	64	0.654	0.856	19.909	0.602	3	136	2	139	93	1 duplicate
11308	21 [678]: N,N-Di-(2-Hydroxy	14 Succinic acid	64	0.636	0.832	10.537	0.541	4	137	4	137	25	30 duplicate
2651	21 [678]: N,N-Di-(2-Hydroxy	[812]: D-Xylofuranose (4TMS)]	62	0.615	0.781	3.759	0.544	5	135	12	129	2	27 original
2714	21 [678]: N,N-Di-(2-Hydroxy	[892]: Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	0.615	0.660	17.207	0.505	6	136	39	102	71	55 original
2629	21 [678]: N,N-Di-(2-Hydroxy	26 Citramalic acid	64	0.615	0.831	2.896	0.534	7	134	5	136	1	34 original
2615	21 [678]: N,N-Di-(2-Hydroxy	40 [680]: 2,3-Dimethylsuccinic acid (2TMS)]	64	0.600	0.805	19.105	0.540	8	133	9	132	88	31 original
11437	21 [678]: N,N-Di-(2-Hydroxy	12 Glycetic acid	63	0.585	0.817	22.025	0.572	9	132	7	134	107	10 duplicate
2627	21 [678]: N,N-Di-(2-Hydroxy	38 [708]: 2,3-Dimethylsuccinic acid (2TMS)]	64	0.581	0.820	11.040	0.585	10	131	6	135	29	3 original
2704	21 [678]: N,N-Di-(2-Hydroxy	115 Glucose-6-phosphate	62	0.568	0.698	9.797	0.537	11	130	30	111	22	33 original
2613	21 [678]: N,N-Di-(2-Hydroxy	24 [725]: 2-Ketooctanoic acid (2TMS)]	64	0.566	0.788	16.613	0.570	12	129	11	130	66	13 original
2618	21 [678]: N,N-Di-(2-Hydroxy	29 Erythritol	64	0.563	0.806	14.631	0.561	13	128	8	133	50	20 original
21943	21 [678]: N,N-Di-(2-Hydroxy	[783]: D-Galactono-1,4-lactone (4TMS)]	61	0.563	0.749	16.351	0.564	14	127	19	122	64	17 original
2665	21 [678]: N,N-Di-(2-Hydroxy	[644]: 2-Methyl-1,3-butanediol (2TMS)]	64	0.559	0.795	4.180	0.562	15	126	10	131	3	19 duplicate
2659	21 [678]: N,N-Di-(2-Hydroxy	70 [693]: 2-Furan-2-hydroxyacetic acid (2TMS)]	64	0.557	0.704	11.884	0.513	16	125	29	112	34	47 original
2695	21 [678]: N,N-Di-(2-Hydroxy	108 [733]: Threitol (4TMS)]	57	0.550	0.500	6.695	0.440	17	124	54	87	9	91 original
2628	21 [678]: N,N-Di-(2-Hydroxy	39 [829]: 1-Phenylethanol (1TMS)]	62	0.542	0.735	12.851	0.541	18	123	23	118	36	29 original
2611	21 [678]: N,N-Di-(2-Hydroxy	22 [690]: N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	63	0.538	0.778	10.976	0.570	19	122	13	128	28	11 original
2654	21 [678]: N,N-Di-(2-Hydroxy	65 [646]: 3-Deoxyglucitol (5TMS)]	52	0.531	0.759	21.830	0.519	20	121	16	125	105	44 original
2689	21 [678]: N,N-Di-(2-Hydroxy	100 [857]: Mannitol (6TMS)]	63	0.529	0.763	20.111	0.569	21	120	15	126	96	15 original
2639	21 [678]: N,N-Di-(2-Hydroxy	50 [746]: Ribonic acid-1,4-lactone (3TMS)]	64	0.528	0.686	9.399	0.495	22	119	35	106	20	60 original
2635	21 [678]: N,N-Di-(2-Hydroxy	46 Arabinose	61	0.521	0.752	30.094	0.513	23	118	18	123	136	49 original
2643	21 [678]: N,N-Di-(2-Hydroxy	54 [NA]	64	0.520	0.748	13.632	0.567	24	117	20	121	43	16 original
2721	21 [678]: N,N-Di-(2-Hydroxy	[895]: Isomaltose methoxyamine (8TMS)]	55	0.518	0.711	21.388	0.526	25	116	28	113	102	38 original
2709	21 [678]: N,N-Di-(2-Hydroxy	120 [945]: Uridine (3TMS)]	42	0.517	0.741	23.791	0.531	26	115	22	119	112	36 original
11565	21 [678]: N,N-Di-(2-Hydroxy	13 Uracil	54	0.511	0.457	6.736	0.548	27	114	58	83	11	26 original
2624	21 [678]: N,N-Di-(2-Hydroxy	35 Pyroglyutamic acid	64	0.511	0.772	6.589	0.569	28	113	14	127	8	14 duplicate
2701	21 [678]: N,N-Di-(2-Hydroxy	[877]: beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	64	0.507	0.669	25.896	0.483	29	112	37	104	120	66 original
2723	21 [678]: N,N-Di-(2-Hydroxy	134 Isomaltose	63	0.506	0.714	28.293	0.476	30	111	27	114	130	70 original
2667	21 [678]: N,N-Di-(2-Hydroxy	78 Mannose	64	0.501	0.758	12.964	0.582	31	110	17	124	38	4 original
12067	21 [678]: N,N-Di-(2-Hydroxy	17 [700]: 2-methyl-1,2-propanediol (2TMS)]	62	0.501	0.689	19.319	0.484	32	109	33	108	91	64 original
2645	21 [678]: N,N-Di-(2-Hydroxy	56 [829]: Orolic acid (3TMS)]	64	0.500	0.727	5.710	0.492	33	108	25	116	5	61 duplicate
2691	21 [678]: N,N-Di-(2-Hydroxy	102 [904]: Galactose methoxyamine (5TMS)]	64	0.496	0.745	19.193	0.573	34	107	21	120	89	9 original
		129 [840]: Galactose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	64	0.486	0.636	16.824	0.516	35	106	43	98	69	46 original
2718	21 [678]: N,N-Di-(2-Hydroxy	88 Gluconic acid	59	0.482	0.717	16.678	0.525	36	105	26	115	68	41 original
2677	21 [678]: N,N-Di-(2-Hydroxy	117 [724]: Glycerol (3TMS)]	64	0.480	0.732	10.536	0.554	37	104	24	117	24	24 original
2710	21 [678]: N,N-Di-(2-Hydroxy	121 [657]: Erythritol (4TMS)]	56	0.478	0.686	16.335	0.513	38	103	34	107	63	48 original
2711	21 [678]: N,N-Di-(2-Hydroxy	122 [644]: Erythritol (4TMS)]	55	0.468	0.653	24.297	0.525	39	102	41	100	114	40 original
2663	21 [678]: N,N-Di-(2-Hydroxy	74 [912]: Tetradecanoic acid (1TMS)]	52	0.468	0.690	25.008	0.523	40	101	32	109	117	42 original
2662	21 [678]: N,N-Di-(2-Hydroxy	73 [708]: Glucose methoxyamine (5TMS)]	64	0.465	0.668	17.424	0.481	41	100	38	103	75	68 original
			57	0.465	0.638	17.676	0.465	42	99	42	99	77	75 original

2646	21	[678; N,N-Di-(2-Hydroxy	[757; 2-Desoxy-pentao-3-yose dimethoxyamine (2TMS)]	55	0.463	0.692	14.571	0.558	43	98	31	110	49	23	original
2724	21	[678; N,N-Di-(2-Hydroxy	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	0.449	0.654	5.650	0.485	44	97	40	101	4	62	original
12312	21	[678; N,N-Di-(2-Hydroxy	Alanine (BP) (3TMS)	64	0.438	0.633	7.871	0.455	45	96	45	96	13	79	duplicate
2633	21	[678; N,N-Di-(2-Hydroxy	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	0.438	0.610	13.212	0.533	46	95	49	92	41	35	original
2703	21	[678; N,N-Di-(2-Hydroxy	Fructose-6-phosphate	53	0.415	0.635	18.386	0.389	47	94	44	97	83	121	original
2702	21	[678; N,N-Di-(2-Hydroxy	Galactose-6-phosphate	62	0.411	0.619	18.161	0.401	48	93	47	94	80	114	original
2699	21	[678; N,N-Di-(2-Hydroxy	[715; Erythritol (4TMS)]	54	0.407	0.614	19.957	0.593	49	92	48	93	94	2	original
2715	21	[678; N,N-Di-(2-Hydroxy	[559; Erythritol (4TMS)]	45	0.398	0.490	16.632	0.560	50	91	56	85	67	21	original
2681	21	[678; N,N-Di-(2-Hydroxy	[680; Glycerol-2-phosphate (4TMS)]	54	0.368	0.526	15.682	0.456	51	90	52	89	61	78	original
2692	21	[678; N,N-Di-(2-Hydroxy	[648; Ethylamine (2TMS)]	63	0.365	0.536	15.123	0.476	52	89	51	90	56	69	original
2674	21	[678; N,N-Di-(2-Hydroxy	[529; Methylcitric acid (4TMS)]	48	0.355	0.670	11.637	0.519	53	88	36	105	33	43	original
2630	21	[678; N,N-Di-(2-Hydroxy	[639; Proline (2TMS)]	64	0.354	0.537	5.719	0.440	54	87	50	91	6	90	original
2685	21	[678; N,N-Di-(2-Hydroxy	myo-Inositol	49	0.330	0.317	29.358	0.317	55	86	74	67	134	139	original
10648	21	[678; N,N-Di-(2-Hydroxy	Glycerol	64	0.321	0.495	26.512	0.389	56	85	55	88	123	120	duplicate
2676	21	[678; N,N-Di-(2-Hydroxy	[945; beta-D-Glucopyranose (5TMS)]	62	0.321	0.501	21.137	0.424	57	84	53	88	101	99	original
2693	21	[678; N,N-Di-(2-Hydroxy	[795; Erythritol (4TMS)]	63	0.311	0.440	14.482	0.416	58	83	60	81	48	103	original
2690	21	[678; N,N-Di-(2-Hydroxy	[832; Dopamine (4TMS)]	64	0.297	0.420	14.693	0.410	59	82	63	78	52	110	original
2705	21	[678; N,N-Di-(2-Hydroxy	[882; Pseudouridine (5TMS)]	30	0.292	0.381	14.391	0.507	60	81	68	73	47	52	original
2688	21	[678; N,N-Di-(2-Hydroxy	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	0.290	0.631	19.292	0.500	61	80	46	95	90	58	original
2712	21	[678; N,N-Di-(2-Hydroxy	[945; Galactofuranose-6-phosphate (7TMS)]	64	0.284	0.400	7.973	0.413	62	79	65	76	14	107	original
2717	21	[678; N,N-Di-(2-Hydroxy	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.267	0.454	11.360	0.503	63	78	59	82	31	58	original
2694	21	[678; N,N-Di-(2-Hydroxy	[705; 2-Ketogluconic acid (5TMS)]	48	0.266	0.458	13.078	0.507	64	77	57	84	40	53	original
2680	21	[678; N,N-Di-(2-Hydroxy	[766; beta-D-Methylglucopyranoside (4TMS)]	64	0.261	0.397	18.762	0.405	65	76	66	75	86	111	original
2686	21	[678; N,N-Di-(2-Hydroxy	[756; beta-D-Methylglucopyranoside (4TMS)]	52	0.249	0.438	14.209	0.450	66	75	62	79	45	80	original
2700	21	[678; N,N-Di-(2-Hydroxy	[11583; Erythritol (4TMS)]	42	0.247	0.388	29.868	0.389	67	74	71	70	135	123	original
2672	21	[678; N,N-Di-(2-Hydroxy	Sorbitol	58	0.235	-0.163	10.711	0.398	68	73	92	49	27	117	original
2729	21	[678; N,N-Di-(2-Hydroxy	[692; Ergosta-7,22-dien-3-ol (1TMS)]	49	0.233	0.350	25.634	0.418	69	72	73	68	119	101	original
2716	21	[678; N,N-Di-(2-Hydroxy	[777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.209	0.384	13.058	0.468	70	71	67	74	39	73	original
2653	21	[678; N,N-Di-(2-Hydroxy	[789; Tyramine (3TMS)]	63	0.203	0.236	15.452	0.370	71	70	77	64	60	130	original
2722	21	[678; N,N-Di-(2-Hydroxy	[855; Squalene]	64	0.188	0.149	14.249	0.378	72	69	80	61	48	127	original
2673	21	[678; N,N-Di-(2-Hydroxy	Mannitol	62	0.194	0.354	18.162	0.426	73	68	72	69	81	97	original
2669	21	[678; N,N-Di-(2-Hydroxy	[772; D-Glucose (5TMS)]	62	0.193	0.403	17.215	0.380	74	67	64	77	72	125	original
2698	21	[678; N,N-Di-(2-Hydroxy	Octadecanoic acid	64	0.159	0.440	12.119	0.418	75	66	61	80	35	102	original
2727	21	[678; N,N-Di-(2-Hydroxy	[674; Ergosterol (1TMS)]	46	0.150	0.261	25.993	0.337	76	65	76	65	121	136	original
11818	21	[678; N,N-Di-(2-Hydroxy	Alanine	64	0.148	0.190	7.750	0.509	77	64	79	62	12	51	duplicate
2668	21	[678; N,N-Di-(2-Hydroxy	Glucose	64	0.145	0.380	20.114	0.475	78	63	69	72	97	72	original
9963	21	[678; N,N-Di-(2-Hydroxy	[938; Sulfuric acid (2TMS)]	36	0.117	0.282	15.344	0.429	79	62	75	66	59	94	duplicate
2683	21	[678; N,N-Di-(2-Hydroxy	Hexadecanoic acid	64	0.114	0.377	9.038	0.413	80	61	70	71	18	106	original
2730	21	[678; N,N-Di-(2-Hydroxy	[141; Lanosta-8,24-dien-3-beta-ol	61	0.106	0.211	24.770	0.446	81	60	78	63	116	85	original
2728	21	[678; N,N-Di-(2-Hydroxy	[700; Ergosta-5,7-dien-3-ol]	38	0.073	-0.004	27.278	0.285	82	59	86	55	126	140	original
2726	21	[678; N,N-Di-(2-Hydroxy	Ergosterol	64	0.051	0.060	11.079	0.425	83	58	82	59	30	98	original
2679	21	[678; N,N-Di-(2-Hydroxy	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	64	0.022	0.047	12.867	0.361	84	57	83	58	37	132	original
2660	21	[678; N,N-Di-(2-Hydroxy	[731; Erythrose (3TMS)]	64	0.019	-0.016	6.725	0.388	85	56	87	54	10	124	original
2707	21	[678; N,N-Di-(2-Hydroxy	[928; Glucopyranose-6-phosphate (6TMS)]	58	0.008	0.068	18.541	0.372	86	55	81	60	84	128	original
2636	21	[678; N,N-Di-(2-Hydroxy	[NA]	64	0.000	-0.024	17.048	0.398	87	54	88	53	70	118	original
2708	21	[678; N,N-Di-(2-Hydroxy	[931; myo-Inositol-2-phosphate (7TMS)]	64	-0.016	0.022	13.713	0.429	88	53	84	57	44	95	original
2642	21	[678; N,N-Di-(2-Hydroxy	Glycerol-2-phosphate	64	-0.036	-0.117	22.482	0.346	89	52	90	51	109	135	original
2625	21	[678; N,N-Di-(2-Hydroxy	[596; N-Acetylglutamic acid (2TMS)]	64	-0.049	-0.278	15.181	0.446	90	51	97	44	57	86	original
2696	21	[678; N,N-Di-(2-Hydroxy	[9-(Z)-Octadecenoic acid	64	-0.062	-0.098	6.197	0.370	91	50	89	52	7	129	original

2682	21	[678; N,N-Di-(2-Hydroxy	93	[607; Putrescine (4TMS)]	60	-0.066	-0.002	27.709	0.402	92	48	85	56	127	113	original
2713	21	[678; N,N-Di-(2-Hydroxy	124	[734; 1-Monoolcylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	59	-0.074	-0.223	35.082	0.379	93	48	85	46	140	126	original
2661	21	[678; N,N-Di-(2-Hydroxy	72	[919; D-Xylopyranose (4TMS)]	63	-0.095	-0.142	19.004	0.324	94	47	91	50	87	138	original
2719	21	[678; N,N-Di-(2-Hydroxy	130	Trehalose	63	-0.116	-0.211	15.258	0.389	95	46	94	47	58	122	original
2725	21	[678; N,N-Di-(2-Hydroxy	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.132	-0.208	8.821	0.334	96	45	93	48	17	137	original
10377	21	[678; N,N-Di-(2-Hydroxy	4	Phosphoric acid	51	-0.153	-0.209	20.606	0.360	97	44	100	41	99	133	duplicate
2697	21	[678; N,N-Di-(2-Hydroxy	108	Oxalacetic acid	64	-0.180	-0.249	18.078	0.364	98	43	96	45	79	131	original
2647	21	[678; N,N-Di-(2-Hydroxy	58	[636; 4R-Acetamidido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	-0.203	-0.362	9.939	0.393	99	42	102	39	23	119	original
2664	21	[678; N,N-Di-(2-Hydroxy	75	Lysine	64	-0.218	-0.438	25.280	0.404	100	41	104	37	118	112	original
2649	21	[678; N,N-Di-(2-Hydroxy	80	Glycerol-3-phosphate	64	-0.226	-0.297	8.540	0.416	101	40	99	42	16	104	original
2656	21	[678; N,N-Di-(2-Hydroxy	67	Citric acid	64	-0.234	-0.344	9.514	0.349	102	39	101	40	21	134	original
10782	21	[678; N,N-Di-(2-Hydroxy	7	Threonine	64	-0.247	-0.407	15.721	0.399	103	38	103	38	62	115	duplicate
2655	21	[678; N,N-Di-(2-Hydroxy	66	Glyceral acid-3-phosphate	64	-0.250	-0.443	17.554	0.449	104	37	105	36	76	81	original
2687	21	[678; N,N-Di-(2-Hydroxy	98	[697; Ribose-5-phosphate methoxamine (5TMS)]	48	-0.266	-0.562	28.515	0.517	105	36	115	26	131	45	original
2641	21	[678; N,N-Di-(2-Hydroxy	52	[NA]	64	-0.268	-0.483	28.635	0.482	106	35	107	34	132	67	original
2650	21	[678; N,N-Di-(2-Hydroxy	61	[NA]	64	-0.274	-0.286	14.670	0.411	107	34	98	43	51	109	original
2652	21	[678; N,N-Di-(2-Hydroxy	63	Glutamine	52	-0.282	-0.541	24.086	0.460	108	33	111	30	113	77	original
2616	21	[678; N,N-Di-(2-Hydroxy	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	-0.309	-0.793	28.060	0.560	109	32	139	2	128	22	original
2626	21	[678; N,N-Di-(2-Hydroxy	37	Phenylalanine	64	-0.313	-0.460	9.126	0.427	110	31	106	35	19	96	original
2644	21	[678; N,N-Di-(2-Hydroxy	55	[612; 4-Aminobutyric acid (2TBS)]	43	-0.333	-0.511	30.331	0.442	111	29	108	33	137	89	original
2632	21	[678; N,N-Di-(2-Hydroxy	43	[548; Leucine (2TBS)]	60	-0.333	-0.530	13.225	0.415	112	30	110	31	42	105	original
2640	21	[678; N,N-Di-(2-Hydroxy	51	[498; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.362	-0.547	28.102	0.485	113	28	113	28	129	59	original
10102	21	[678; N,N-Di-(2-Hydroxy	3	Serine	62	-0.382	-0.552	16.560	0.447	114	27	114	27	65	84	duplicate
10240	21	[678; N,N-Di-(2-Hydroxy	3	Ethanolamine	62	-0.396	-0.589	22.329	0.444	115	26	116	25	108	87	duplicate
2720	21	[678; N,N-Di-(2-Hydroxy	131	[826; 5-Methylthiadenosine (3TMS)]	55	-0.414	-0.542	27.132	0.476	116	25	112	29	125	71	original
2621	21	[678; N,N-Di-(2-Hydroxy	32	[729; N,N-Dimethyllysine methyl ester]	63	-0.430	-0.718	26.332	0.564	117	24	130	11	122	18	original
10915	21	[678; N,N-Di-(2-Hydroxy	8	Isoleucine	55	-0.440	-0.515	14.927	0.399	118	23	109	32	54	116	duplicate
2684	21	[678; N,N-Di-(2-Hydroxy	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	-0.442	-0.591	28.911	0.442	119	22	117	24	133	88	original
2657	21	[678; N,N-Di-(2-Hydroxy	68	[570; Hypoxanthine (2TMS)]	20	-0.442	-0.791	20.812	0.421	120	21	138	3	100	100	original
2612	21	[678; N,N-Di-(2-Hydroxy	23	Homoserine	64	-0.443	-0.800	17.228	0.581	121	20	140	1	73	5	original
2670	21	[678; N,N-Di-(2-Hydroxy	81	Tyrosine	64	-0.447	-0.625	21.802	0.483	122	19	119	22	104	65	original
2678	21	[678; N,N-Di-(2-Hydroxy	89	[775; Dopamine (4TMS)]	35	-0.449	-0.655	22.743	0.411	123	18	122	19	111	108	original
2620	21	[678; N,N-Di-(2-Hydroxy	31	[822; Parabenic acid (2TMS)]	64	-0.456	-0.686	22.519	0.503	124	17	126	15	110	57	original
2637	21	[678; N,N-Di-(2-Hydroxy	48	Asparagine	64	-0.464	-0.684	18.354	0.506	125	16	125	16	82	54	original
11047	21	[678; N,N-Di-(2-Hydroxy	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.473	-0.775	24.345	0.527	126	15	135	6	115	37	original
2638	21	[678; N,N-Di-(2-Hydroxy	9	Proline	63	-0.481	-0.618	20.164	0.448	127	14	118	23	98	82	duplicate
12433	21	[678; N,N-Di-(2-Hydroxy	49	[877; Pyrophosphoric acid (4TMS)]	64	-0.495	-0.628	31.937	0.434	128	13	120	21	138	93	original
2658	21	[678; N,N-Di-(2-Hydroxy	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.497	-0.744	21.911	0.574	129	12	132	9	106	8	duplicate
2648	21	[678; N,N-Di-(2-Hydroxy	59	Arginine	60	-0.499	-0.783	15.104	0.570	130	11	136	5	55	12	original
2634	21	[678; N,N-Di-(2-Hydroxy	45	Ornithine; Arginine	64	-0.500	-0.643	26.740	0.466	131	10	121	20	124	74	original
11178	21	[678; N,N-Di-(2-Hydroxy	10	Glycine	61	-0.502	-0.694	33.320	0.447	132	9	127	14	139	83	original
2666	21	[678; N,N-Di-(2-Hydroxy	82	benzeneacetic acid methyl ester]	64	-0.508	-0.755	11.612	0.576	133	8	134	7	32	7	duplicate
2671	21	[678; N,N-Di-(2-Hydroxy	82	Lysine	62	-0.508	-0.681	19.971	0.462	134	7	123	18	95	76	original
2631	21	[678; N,N-Di-(2-Hydroxy	42	Glutamic acid	39	-0.522	-0.785	14.780	0.511	135	6	137	4	53	50	original
2623	21	[678; N,N-Di-(2-Hydroxy	34	Aspartic acid	60	-0.525	-0.695	21.724	0.484	136	5	129	12	103	63	original
2622	21	[678; N,N-Di-(2-Hydroxy	33	Methionine	64	-0.529	-0.694	19.769	0.525	137	4	128	13	92	39	original
					64	-0.530	-0.721	17.313	0.537	138	3	131	10	74	32	original

2619	21	[678; N,N-Di-(2-Hydroxy	30	[815; Ethyl-3(2H)-thiophenone]	64	-0.538	-0.684	18,758	0.439	139	2	124	17	85	92 original
10513	21	[678; N,N-Di-(2-Hydroxy	5	Leucine	45	-0.543	-0.755	17,856	0.543	140	1	133	8	78	28 duplicate
2736	22	[690; N,N-Di-(2-Hydroxy	28	Malic acid	52	0.710	0.940	14,610	0.610	1	140	2	139	70	20 original
11693	22	[690; N,N-Di-(2-Hydroxy	14	Fumaric acid	52	0.674	0.925	5,189	0.614	2	139	5	136	6	18 duplicate
11309	22	[690; N,N-Di-(2-Hydroxy	11	Succinic acid	52	0.667	0.887	13,124	0.607	3	138	14	127	59	25 duplicate
11944	22	[690; N,N-Di-(2-Hydroxy	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	52	0.638	0.923	22,838	0.622	4	137	6	135	103	9 duplicate
2747	22	[690; N,N-Di-(2-Hydroxy	39	[828; 1-Phenylethanol (1TMS)]	52	0.637	0.929	18,668	0.619	5	136	4	137	89	13 original
2754	22	[690; N,N-Di-(2-Hydroxy	46	Arafinose	52	0.633	0.877	19,322	0.621	6	135	18	123	83	10 original
2762	22	[690; N,N-Di-(2-Hydroxy	54	[NA]	46	0.629	0.853	4,640	0.551	7	134	21	120	4	52 original
2824	22	[690; N,N-Di-(2-Hydroxy	24	[725; 2-Ketobutanoic acid (2TMS)]	52	0.627	0.921	36,070	0.620	8	133	7	134	129	12 original
2734	22	[690; N,N-Di-(2-Hydroxy	26	Citramalic acid	25	0.627	0.643	7,072	0.322	9	132	52	89	15	138 original
2748	22	[690; N,N-Di-(2-Hydroxy	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	52	0.626	0.867	21,978	0.562	10	130	19	122	99	45 original
2746	22	[690; N,N-Di-(2-Hydroxy	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	52	0.623	0.850	38,564	0.602	11	131	22	119	134	28 original
2770	22	[690; N,N-Di-(2-Hydroxy	62	[812; D-Xylofuranose (4TMS)]	52	0.623	0.945	12,331	0.625	12	128	1	140	53	6 original
2764	22	[690; N,N-Di-(2-Hydroxy	56	[829; Orolic acid (3TMS)]	52	0.612	0.887	8,180	0.598	14	127	28	113	94	26 original
2823	22	[690; N,N-Di-(2-Hydroxy	115	Glucose-6-phosphate	52	0.609	0.749	29,908	0.582	15	126	40	101	119	31 original
2794	22	[690; N,N-Di-(2-Hydroxy	65	[793; D-Galactono-1,4-lactone (4TMS)]	51	0.605	0.838	23,891	0.648	16	125	26	115	105	1 original
2773	22	[690; N,N-Di-(2-Hydroxy	57	[646; 3-Deoxyglucitol (5TMS)]	52	0.602	0.907	9,688	0.613	17	124	10	131	32	19 original
2765	22	[690; N,N-Di-(2-Hydroxy		[757; 2-Desoxy-pentose-3-yose dimethoxamine (2TMS)]	47	0.600	0.845	14,116	0.626	18	123	25	116	68	5 original
11566	22	[690; N,N-Di-(2-Hydroxy	13	Uracil	52	0.599	0.916	20,249	0.623	19	122	8	133	96	7 duplicate
2842	22	[690; N,N-Di-(2-Hydroxy	134	Isomaltose	52	0.593	0.902	28,247	0.639	20	121	36	105	118	3 original
2784	22	[690; N,N-Di-(2-Hydroxy	78	Fructose	52	0.593	0.764	28,745	0.573	21	121	3	136	105	40 original
2814	22	[690; N,N-Di-(2-Hydroxy	106	[733; Threitol (4TMS)]	51	0.589	0.813	12,827	0.601	22	119	29	112	58	28 original
2837	22	[690; N,N-Di-(2-Hydroxy		[640; Malibose methoxamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	52	0.588	0.881	10,626	0.570	23	118	17	124	39	41 original
2737	22	[690; N,N-Di-(2-Hydroxy	89	Erythritol	52	0.585	0.915	9,574	0.627	24	116	9	132	30	4 original
2796	22	[690; N,N-Di-(2-Hydroxy	88	Gluconic acid	52	0.585	0.858	15,279	0.618	25	117	20	121	73	15 original
2743	22	[690; N,N-Di-(2-Hydroxy	35	Pyrogulamic acid	52	0.582	0.740	45,260	0.542	26	115	42			

2782	22 [690; N,N-Di-(2-Hydroxy 74 [912; Tetradecanoic acid (1TMS)]	52	0.468	0.711	9.791	0.530	47	94	47	94	33	61	original
2828	22 [690; N,N-Di-(2-Hydroxy 120 [945; Uridine (3TMS)]	48	0.458	0.282	17.396	0.609	48	93	78	63	82	21	original
2752	22 [690; N,N-Di-(2-Hydroxy 44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	42	0.449	0.741	10.203	0.607	49	92	41	100	37	24	original
2813	22 [690; N,N-Di-(2-Hydroxy 105 [705; 2-Ketogluconic acid (5TMS)]	42	0.440	0.756	12.228	0.567	50	91	38	103	52	43	original
12191	22 [690; N,N-Di-(2-Hydroxy 18 [590; 1-Acetyl-2-thiodyantoin]	52	0.416	0.580	13.293	0.457	51	90	59	82	62	87	Jupicate
2805	22 [690; N,N-Di-(2-Hydroxy 97 [756; beta-D-Methylglucopyranoside (4TMS)]	46	0.414	0.655	22.466	0.487	52	89	50	91	100	73	original
2836	22 [690; N,N-Di-(2-Hydroxy 128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	39	0.409	0.801	9.806	0.607	53	88	32	109	34	23	original
2809	22 [690; N,N-Di-(2-Hydroxy 101 [832; Dopamine (4TMS)]	52	0.409	0.628	13.205	0.450	54	87	53	88	61	91	original
2822	22 [690; N,N-Di-(2-Hydroxy 114 Fructose-6-phosphate	45	0.408	0.648	6.063	0.485	55	86	51	80	9	83	original
2834	22 [690; N,N-Di-(2-Hydroxy 126 [559; Erythritol (4TMS)]	40	0.408	0.680	5.828	0.615	56	85	49	92	8	17	original
2821	22 [690; N,N-Di-(2-Hydroxy 113 Galactose-6-phosphate	52	0.395	0.588	8.612	0.440	57	84	56	85	25	95	original
12313	22 [690; N,N-Di-(2-Hydroxy 19 Alanine (BP) (3TMS)	52	0.394	0.578	17.212	0.469	58	83	60	81	80	81	Jupicate
2835	22 [690; N,N-Di-(2-Hydroxy 127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	34	0.376	0.835	5.242	0.617	59	82	27	114	7	16	original
2795	22 [690; N,N-Di-(2-Hydroxy 87 [945; beta-D-Glucopyranose (5TMS)]	50	0.355	0.581	38.540	0.442	60	81	58	83	132	94	original
2789	22 [690; N,N-Di-(2-Hydroxy 91 [768; beta-D-Methylglucopyranoside (4TMS)]	52	0.354	0.592	17.412	0.437	61	80	55	86	83	99	original
2848	22 [690; N,N-Di-(2-Hydroxy 140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	38	0.351	0.473	6.776	0.418	62	79	64	77	12	113	original
2804	22 [690; N,N-Di-(2-Hydroxy 98 myo-Inositol	38	0.346	0.296	9.404	0.268	63	78	75	66	28	140	original
2749	22 [690; N,N-Di-(2-Hydroxy 41 [639; Proline (2TMS)]	52	0.344	0.516	19.110	0.401	64	77	62	79	92	121	original
2807	22 [690; N,N-Di-(2-Hydroxy 99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	35	0.334	0.892	4.086	0.621	65	76	13	128	2	11	original
10849	22 [690; N,N-Di-(2-Hydroxy 6 Glycerol	52	0.293	0.463	45.559	0.482	66	75	65	78	140	74	Jupicate
2831	22 [690; N,N-Di-(2-Hydroxy 123 [945; Galactofuranose-6-phosphate (7TMS)]	52	0.291	0.342	16.940	0.518	67	74	71	70	78	68	original
2819	22 [690; N,N-Di-(2-Hydroxy 139 [583; Erythritol (4TMS)]	30	0.260	0.322	11.537	0.436	68	73	73	68	47	100	original
2847	22 [690; N,N-Di-(2-Hydroxy 111 [700; Ergosta-5,7-dien-3-ol]	36	0.251	0.301	10.155	0.463	69	72	74	67	36	85	original
2791	22 [690; N,N-Di-(2-Hydroxy 83 Sorbitol	46	0.233	-0.254	26.885	0.327	70	71	94	47	112	136	original
2817	22 [690; N,N-Di-(2-Hydroxy 109 Octadecanoic acid	52	0.228	0.493	25.858	0.417	71	70	63	78	110	114	original
2788	22 [690; N,N-Di-(2-Hydroxy 80 [772; D-Glucose (5TMS)]	50	0.208	0.447	34.585	0.417	72	69	68	73	122	116	original
2812	22 [690; N,N-Di-(2-Hydroxy 104 [795; Erythritol (4TMS)]	51	0.194	0.343	11.539	0.446	73	68	70	71	48	92	original
2846	22 [690; N,N-Di-(2-Hydroxy 138 [674; Ergosterol (1TMS)]	37	0.192	0.247	8.546	0.408	74	67	81	60	24	118	original
2792	22 [690; N,N-Di-(2-Hydroxy 84 Mannitol	50	0.190	0.527	35.538	0.434	75	66	61	80	126	101	original
2802	22 [690; N,N-Di-(2-Hydroxy 94 Hexadecanoic acid	52	0.184	0.458	26.092	0.463	76	65	66	75	111	86	original
2849	22 [690; N,N-Di-(2-Hydroxy 141 Lanosta-8,24-dien-3-beta-ol	50	0.177	0.331	7.176	0.427	77	64	72	69	17	105	original
2841	22 [690; N,N-Di-(2-Hydroxy 133 [855; Squalene]	52	0.172	0.122	12.762	0.383	78	63	83	58	57	128	original
2755	22 [690; N,N-Di-(2-Hydroxy 47 [NA]	52	0.157	0.223	13.558	0.422	79	62	82	59	63	108	original
2798	22 [690; N,N-Di-(2-Hydroxy 90 [910; 9-(Z)-Hexadecanoic acid (1TMS)]	52	0.133	0.292	12.455	0.381	80	61	77	64	55	128	original
8964	22 [690; N,N-Di-(2-Hydroxy 1 [938; Sulfuric acid (2TMS)]	30	0.122	0.455	6.806	0.579	81	60	67	74	13	39	Jupicate
2845	22 [690; N,N-Di-(2-Hydroxy 137 Ergosterol	52	0.100	0.097	18.951	0.401	82	59	86	55	91	122	original
2801	22 [690; N,N-Di-(2-Hydroxy 93 [607; Putrescine (4TMS)]	49	0.094	0.295	9.019	0.374	83	58	76	65	26	131	original
2772	22 [690; N,N-Di-(2-Hydroxy 64 [789; Tyramine (3TMS)]	52	0.089	0.033	10.677	0.423	84	57	87	54	42	107	original
2826	22 [690; N,N-Di-(2-Hydroxy 118 [928; Glucopyranose-6-phosphate (6TMS)]	51	0.078	0.105	10.629	0.360	85	56	85	58	40	132	original
2827	22 [690; N,N-Di-(2-Hydroxy 119 [931; myo-Inositol-2-phosphate (7TMS)]	52	0.063	0.271	12.333	0.489	86	55	79	62	54	70	original
2815	22 [690; N,N-Di-(2-Hydroxy 107 9-(Z)-Octadecanoic acid	52	0.036	0.119	20.178	0.415	87	54	84	57	95	117	original
2761	22 [690; N,N-Di-(2-Hydroxy 53 Glycerol-2-phosphate	52	0.023	0.021	7.246	0.310	88	53	89	52	18	139	original
	124 [734; 1-Monooctylethylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	47	0.008	-0.070	13.670	0.392	89	52	90	51	66	125	original
2832	22 [690; N,N-Di-(2-Hydroxy 15 Alanine	52	-0.008	0.026	25.130	0.580	90	51	88	53	106	38	Jupicate
11819	22 [690; N,N-Di-(2-Hydroxy 79 Glucose	52	-0.017	0.263	39.699	0.530	91	50	80	61	136	60	original
2779	22 [690; N,N-Di-(2-Hydroxy 71 [731; Erythrose (3TMS)]	52	-0.021	-0.106	18.512	0.427	92	49	83	48	88	104	original
2780	22 [690; N,N-Di-(2-Hydroxy 72 [918; D-Xylopyranose (4TMS)]	51	-0.035	-0.077	10.924	0.345	93	48	91	50	43	133	original
2844	22 [690; N,N-Di-(2-Hydroxy 136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	16	-0.050	-0.104	4.155	0.432	94	47	92	49	3	103	original
2760	22 [690; N,N-Di-(2-Hydroxy 52 [NA]	36	-0.098	-0.352	14.955	0.560	95	46	97	44	72	47	original
2838	22 [690; N,N-Di-(2-Hydroxy 130 Trehalose	52	-0.193	-0.340	34.781	0.424	96	45	96	45	123	108	original

2616	22 [690; N,N-Di-(2-Hydroxy	108	Octadecenoic acid	52	-0.198	-0.315	10.443	0.421	97	44	95	46	38	109 original
2771	22 [690; N,N-Di-(2-Hydroxy	63	Glutamine	41	-0.205	-0.534	16.169	0.561	98	43	106	35	76	46 original
2768	22 [690; N,N-Di-(2-Hydroxy	60	Glycerol-3-phosphate	52	-0.240	-0.368	27.365	0.418	99	42	98	43	113	112 original
2775	22 [690; N,N-Di-(2-Hydroxy	67	Citric acid	52	-0.244	-0.428	29.292	0.342	100	41	100	41	117	134 original
2766	22 [690; N,N-Di-(2-Hydroxy	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	52	-0.252	-0.485	22.628	0.395	101	39	102	39	102	123 original
10783	22 [690; N,N-Di-(2-Hydroxy	7	Threonine	52	-0.252	-0.496	35.493	0.437	102	40	104	37	125	97 duplicate
10378	22 [690; N,N-Di-(2-Hydroxy	4	Phosphoric acid	39	-0.255	-0.424	37.388	0.340	103	38	89	42	131	135 duplicate
2769	22 [690; N,N-Di-(2-Hydroxy	61	[NA]	52	-0.264	-0.457	12.561	0.494	104	37	101	40	58	71 original
2744	22 [690; N,N-Di-(2-Hydroxy	36	[596; N-Acetylglutamic acid (2TMS)]	52	-0.297	-0.571	33.806	0.369	105	36	110	31	121	126 original
2751	22 [690; N,N-Di-(2-Hydroxy	43	[548; Leucine (2TBS)]	50	-0.304	-0.480	14.817	0.434	106	35	103	38	71	102 original
2783	22 [690; N,N-Di-(2-Hydroxy	75	Lysine	52	-0.305	-0.559	43.944	0.451	107	34	109	32	137	80 original
2745	22 [690; N,N-Di-(2-Hydroxy	37	Phenylalanine	52	-0.371	-0.579	28.642	0.408	108	33	111	30	116	119 original
2803	22 [690; N,N-Di-(2-Hydroxy	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	40	-0.374	-0.540	12.200	0.374	109	32	107	34	51	130 original
2766	22 [690; N,N-Di-(2-Hydroxy	48	Asparagine	52	-0.428	-0.707	17.528	0.568	110	31	124	17	85	42 original
10103	22 [690; N,N-Di-(2-Hydroxy	2	Serine	51	-0.428	-0.615	25.871	0.420	111	30	115	26	109	110 duplicate
2735	22 [690; N,N-Di-(2-Hydroxy	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	45	-0.432	-0.881	18.763	0.553	112	29	136	5	90	51 original
2774	22 [690; N,N-Di-(2-Hydroxy	66	Glyceric acid-3-phosphate	52	-0.436	-0.702	11.202	0.543	113	27	123	18	45	55 original
2806	22 [690; N,N-Di-(2-Hydroxy	98	[697; Ribose-5-phosphate methoxymethylamine (5TMS)]	39	-0.436	-0.841	13.753	0.548	114	28	132	9	67	53 original
2759	22 [690; N,N-Di-(2-Hydroxy	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	36	-0.444	-0.755	12.091	0.477	115	26	130	11	50	77 original
10241	22 [690; N,N-Di-(2-Hydroxy	3	Ethanolamine	50	-0.450	-0.675	11.635	0.437	116	25	119	22	49	98 duplicate
2753	22 [690; N,N-Di-(2-Hydroxy	45	Homocysteine	51	-0.457	-0.579	13.138	0.451	117	24	112	29	60	89 original
2839	22 [690; N,N-Di-(2-Hydroxy	131	[626; 5-Methylthioadenosine (3TMS)]	44	-0.461	-0.611	10.634	0.473	118	23	114	27	41	79 original
12434	22 [690; N,N-Di-(2-Hydroxy	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	24	-0.464	-0.725	11.351	0.464	119	22	126	15	46	84 duplicate
2739	22 [690; N,N-Di-(2-Hydroxy	31	[622; Parabenic acid (2TMS)]	52	-0.468	-0.754	11.182	0.531	120	21	129	12	44	59 original
2797	22 [690; N,N-Di-(2-Hydroxy	89	[775; Dopamine (4TMS)]	29	-0.468	-0.676	16.472	0.394	121	20	121	20	77	124 original
2757	22 [690; N,N-Di-(2-Hydroxy	49	[877; Pyrophosphoric acid (4TMS)]	52	-0.481	-0.547	15.497	0.453	122	19	108	33	74	88 original
2742	22 [690; N,N-Di-(2-Hydroxy	34	Aspartic acid	52	-0.486	-0.628	38.617	0.527	123	18	116	25	133	63 original
2733	22 [690; N,N-Di-(2-Hydroxy	25	[709; 2,5-Diaminovalerolactam (2TMS)]	42	-0.491	-0.911	17.416	0.598	124	17	139	2	84	30 original
2740	22 [690; N,N-Di-(2-Hydroxy	32	[729; N,N-Dimethyllysine methyl ester]	51	-0.492	-0.800	17.256	0.582	125	16	131	10	81	35 original
11048	22 [690; N,N-Di-(2-Hydroxy	9	Proline	51	-0.495	-0.652	33.778	0.443	126	15	117	24	120	93 duplicate
2785	22 [690; N,N-Di-(2-Hydroxy	77	[826; beta-[[[5-methyl-2-thienyl]methyl]eneamino-benzeneacetic acid methyl ester]	50	-0.499	-0.712	35.339	0.419	127	14	125	16	124	111 original
10916	22 [690; N,N-Di-(2-Hydroxy	8	Isoleucine	45	-0.505	-0.513	25.447	0.322	128	13	105	36	107	137 duplicate
2741	22 [690; N,N-Di-(2-Hydroxy	33	Methionine	52	-0.511	-0.681	17.155	0.527	129	11	118	23	79	64 original
2731	22 [690; N,N-Di-(2-Hydroxy	23	Homoserine	52	-0.511	-0.910	18.135	0.584	130	12	138	3	86	32 original
2789	22 [690; N,N-Di-(2-Hydroxy	81	Tyrosine	52	-0.514	-0.740	38.873	0.539	131	10	128	13	135	58 original
2777	22 [690; N,N-Di-(2-Hydroxy	69	Arginine	50	-0.517	-0.857	28.020	0.581	132	9	133	8	114	37 original
2738	22 [690; N,N-Di-(2-Hydroxy	30	[815; Ethyl-3(2H)-thiophenone]	52	-0.517	-0.675	35.991	0.478	133	8	120	21	128	76 original
2767	22 [690; N,N-Di-(2-Hydroxy	59	Ornithine; Arginine	52	-0.519	-0.895	45.198	0.468	134	7	122	19	138	82 original
2776	22 [690; N,N-Di-(2-Hydroxy	68	[570; Hypoxanthine (2TMS)]	15	-0.524	-0.949	9.673	0.387	135	6	140	1	31	127 original
2763	22 [690; N,N-Di-(2-Hydroxy	55	[612; 4-Aminobutyric acid (2TBS)]	34	-0.547	-0.910	13.645	0.405	136	5	113	28	65	120 original
2750	22 [690; N,N-Di-(2-Hydroxy	42	Glutamic acid	50	-0.554	-0.727	35.577	0.490	137	4	127	14	127	72 original
2790	22 [690; N,N-Di-(2-Hydroxy	82	Lysine	30	-0.588	-0.864	21.359	0.519	138	3	135	6	97	66 original
10514	22 [690; N,N-Di-(2-Hydroxy	5	Leucine	36	-0.622	-0.858	13.598	0.545	139	2	134	7	64	54 duplicate
11179	22 [690; N,N-Di-(2-Hydroxy	10	Glycine	52	-0.653	-0.900	25.730	0.619	140	1	137	4	108	14 duplicate
2894	23 Homoserine	68	[570; Hypoxanthine (2TMS)]	20	0.705	0.953	15.162	0.567	1	140	1	140	56	40 original
11049	23 Homoserine	9	Proline	63	0.679	0.846	22.153	0.505	2	139	26	115	106	63 duplicate
10917	23 Homoserine	8	Isoleucine	55	0.667	0.521	13.808	0.473	3	138	34	107	42	84 duplicate
2857	23 Homoserine	31	[622; Parabenic acid (2TMS)]	64	0.666	0.836	10.781	0.561	4	137	6	135	16	41 original

10104	23 Homoserine	2	Serine	62	0.625	0.603	13,919	0.491	5	136	28	113	44	73 Juplicate
2924	23 Homoserine	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	48	0.599	0.821	19,209	0.594	6	135	8	133	86	25 original
2859	23 Homoserine	33	Methionine	34	0.592	0.678	7,400	0.571	7	134	20	121	4	37 original
2853	23 Homoserine	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	0.589	0.939	15,859	0.659	8	133	2	139	59	3 original
2856	23 Homoserine	30	[815; Ethyl-3(2H)-thiophenone]	64	0.572	0.699	25,089	0.465	9	132	17	124	120	86 original
2851	23 Homoserine	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	0.569	0.924	8,506	0.574	10	131	3	138	5	34 original
2892	23 Homoserine	66	Glyceric acid-3-phosphate	64	0.568	0.687	8,687	0.496	11	130	19	122	7	71 original
11180	23 Homoserine	10	Glycine	64	0.527	0.862	13,706	0.597	12	129	4	137	40	24 Juplicate
2860	23 Homoserine	34	Aspartic acid	64	0.524	0.652	28,768	0.517	13	128	24	117	127	57 original
2885	23 Homoserine	59	Ornithine; Arginine	64	0.505	0.722	37,137	0.502	14	127	14	127	138	66 original
2871	23 Homoserine	45	Homocysteine	61	0.494	0.650	22,768	0.463	15	126	25	116	108	87 original
2858	23 Homoserine	32	[728; N,N-Dimethyllysine methyl ester]	63	0.490	0.801	12,255	0.652	16	125	10	131	24	5 original
2874	23 Homoserine	48	Asparagine	64	0.485	0.749	7,069	0.574	17	124	12	129	3	36 original
2895	23 Homoserine	69	Arginine	60	0.482	0.855	14,536	0.655	18	123	5	136	49	4 original
2915	23 Homoserine	89	[775; Dopamine (4TMS)]	35	0.476	0.687	13,527	0.534	19	122	18	123	38	48 original
10784	23 Homoserine	7	Threonine	64	0.464	0.548	27,053	0.448	20	121	31	110	122	95 Juplicate
2907	23 Homoserine	81	Tyrosine	64	0.454	0.716	29,332	0.554	21	120	15	126	129	42 original
10515	23 Homoserine	5	Leucine	45	0.442	0.815	9,340	0.677	22	119	9	132	8	1 Juplicate
2868	23 Homoserine	42	Glutamic acid	60	0.423	0.736	23,493	0.546	23	118	13	128	112	45 original
2869	23 Homoserine	43	[548; Leucine (2TBS)]	60	0.417	0.628	6,864	0.460	24	117	27	114	2	88 original
2908	23 Homoserine	82	Lysine	39	0.414	0.834	9,960	0.624	25	116	7	134	10	8 original
2863	23 Homoserine	37	Phenylalanine	64	0.413	0.594	19,847	0.473	26	115	29	112	91	82 original
2877	23 Homoserine	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	0.410	0.789	21,560	0.615	27	114	11	130	103	15 original
2903	23 Homoserine	77	[626; beta-[[[5-methyl-2-thienyl]methyl]amino]-benzeneacetic acid methyl ester]	62	0.405	0.704	24,482	0.542	28	113	16	125	115	47 original
10242	23 Homoserine	3	Ethanolamine	62	0.394	0.654	11,484	0.482	29	112	22	119	19	79 Juplicate
2901	23 Homoserine	75	Lysine	64	0.372	0.571	38,153	0.441	30	111	30	111	137	103 original
2957	23 Homoserine	131	[626; 5-Methylthioadenosine (3TMS)]	55	0.366	0.654	17,474	0.502	31	110	21	120	68	67 original
2887	23 Homoserine	61	[NA]	64	0.344	0.391	8,593	0.405	32	109	41	100	6	118 original
2889	23 Homoserine	63	Glutamine	52	0.338	0.545	12,679	0.546	33	108	33	108	30	44 original
2884	23 Homoserine	58	[636; 4R-Acetalamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	0.321	0.514	12,883	0.413	34	107	35	106	32	116 original
2875	23 Homoserine	49	[877; Pyrophosphoric acid (4TMS)]	64	0.306	0.545	19,640	0.446	35	106	32	109	80	97 original
2881	23 Homoserine	55	[612; 4-Aminobutyric acid (2TBS)]	43	0.267	0.468	24,803	0.533	36	105	37	104	117	49 original
2893	23 Homoserine	67	Citric acid	64	0.263	0.449	21,162	0.399	37	104	38	103	100	122 original
2886	23 Homoserine	60	Glycerol-3-phosphate	64	0.237	0.372	18,760	0.495	38	103	42	99	82	72 original
2878	23 Homoserine	52	[NA]	46	0.233	0.438	18,865	0.531	39	102	40	101	84	51 original
2862	23 Homoserine	36	[596; N-Acetylglutamic acid (2TMS)]	64	0.226	0.482	25,200	0.444	40	101	36	105	121	101 original
2921	23 Homoserine	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	0.198	0.447	21,994	0.445	41	100	39	102	105	98 original
2862	23 Homoserine	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.191	0.283	5,303	0.326	42	99	46	95	1	138 original
2958	23 Homoserine	130	Trehalose	63	0.188	0.360	27,180	0.368	43	98	43	98	124	130 original
10379	23 Homoserine	4	Phosphoric acid	51	0.172	0.359	28,833	0.449	44	97	44	97	128	94 Juplicate
12435	23 Homoserine	20	[618; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	31	0.131	0.654	17,050	0.662	45	96	23	118	64	2 Juplicate
2934	23 Homoserine	108	Octadecenoic acid	64	0.121	0.348	10,086	0.375	46	95	45	96	11	128 original
11820	23 Homoserine	15	Alanine	64	0.073	-0.018	17,329	0.571	47	94	55	86	67	38 Juplicate
2909	23 Homoserine	83	Sorbitol	58	0.061	0.233	17,984	0.445	48	93	47	94	73	99 original
2897	23 Homoserine	71	[731; Erythrose (3TMS)]	64	0.060	0.107	11,447	0.431	49	92	49	92	18	106 original
2890	23 Homoserine	64	[788; Tyramine (3TMS)]	63	0.059	-0.009	8,932	0.335	50	91	54	87	9	137 original
2905	23 Homoserine	79	Glucose	64	0.035	-0.253	33,117	0.477	51	90	63	78	135	81 original
9965	23 Homoserine	1	[838; Sulfuric acid (2TMS)]	36	0.003	-0.281	10,572	0.428	52	89	66	75	13	108 Juplicate



2879	23 Homoserine	53 Glycerol-2-phosphate	64 -0.015	0.086	13.887	0.344	53	88	50	91	43	134 original
2880	23 Homoserine	124 [734; 1-Monooctadecylglycerol (2TMS); 1-Monohexadecanoylglycerol (2TMS)]	59 -0.031	0.122	24.628	0.385	54	87	48	93	116	125 original
2881	23 Homoserine	72 [919; D-Xylopyranose (4TMS)]	63 -0.088	0.047	12.629	0.343	55	86	52	89	29	135 original
2882	23 Homoserine	107 9-(Z)-Octadecenoic acid	64 -0.074	0.053	13.463	0.342	56	85	51	90	37	138 original
2883	23 Homoserine	93 [607; Putrescine (4TMS)]	60 -0.120	-0.285	20.042	0.375	57	84	67	74	94	127 original
2884	23 Homoserine	111 [583; Erythritol (4TMS)]	42 -0.122	-0.254	19.440	0.361	58	83	64	77	87	132 original
2885	23 Homoserine	123 [945; Galactofuranose-6-phosphate (7TMS)]	64 -0.128	-0.268	12.117	0.444	59	82	68	73	22	102 original
2886	23 Homoserine	133 [855; Squalene]	64 -0.140	-0.071	11.396	0.397	60	81	56	85	17	123 original
2887	23 Homoserine	119 [931; myo-Inositol-2-phosphate (7TMS)]	64 -0.144	-0.166	11.787	0.402	61	80	60	81	20	119 original
2888	23 Homoserine	118 [928; Glucopyranose-6-phosphate (6TMS)]	58 -0.149	-0.190	13.373	0.372	62	79	61	80	35	128 original
2889	23 Homoserine	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	64 -0.154	-0.137	10.637	0.379	63	78	58	83	14	126 original
2890	23 Homoserine	6 Glycerol	64 -0.158	-0.452	39.480	0.414	64	77	73	68	140	114 duplicate
2891	23 Homoserine	104 [795; Erythritol (4TMS)]	63 -0.163	-0.355	13.080	0.433	65	76	71	70	33	105 original
2892	23 Homoserine	137 Ergosterol	64 -0.167	0.004	14.516	0.390	66	75	53	88	48	124 original
2893	23 Homoserine	139 [700; Ergosta-5,7-dien-3-ol]	38 -0.181	-0.082	17.802	0.274	67	74	57	84	69	140 original
2894	23 Homoserine	47 [NA]	64 -0.188	-0.161	14.678	0.444	68	73	59	82	50	100 original
2895	23 Homoserine	138 [674; Ergosterol (1TMS)]	46 -0.190	-0.225	17.041	0.365	69	72	62	79	63	131 original
2896	23 Homoserine	96 myo-Inositol	49 -0.199	-0.261	21.458	0.305	70	71	65	76	102	139 original
2897	23 Homoserine	113 Galactose-6-phosphate	62 -0.214	-0.538	15.375	0.417	71	70	81	60	57	113 original
2898	23 Homoserine	84 Mannitol	62 -0.229	-0.491	30.979	0.473	72	69	77	64	131	83 original
2899	23 Homoserine	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41 -0.244	-0.791	14.207	0.497	73	68	120	21	47	70 original
2900	23 Homoserine	94 Hexadecanoic acid	64 -0.244	-0.424	21.734	0.402	74	67	72	69	104	120 original
2901	23 Homoserine	73 [708; Glucose methoxyamine (5TMS)]	57 -0.246	-0.595	17.708	0.507	75	66	89	52	71	60 original
2902	23 Homoserine	80 [772; D-Glucose (5TMS)]	62 -0.251	-0.452	30.126	0.429	76	65	74	67	130	107 original
2903	23 Homoserine	109 Octadecanoic acid	64 -0.261	-0.470	23.954	0.413	77	64	75	66	113	115 original
2904	23 Homoserine	114 Fructose-6-phosphate	53 -0.261	-0.584	14.137	0.424	78	63	88	53	46	111 original
2905	23 Homoserine	91 [766; beta-D-Methylglucopyranoside (4TMS)]	64 -0.266	-0.536	23.155	0.484	79	62	80	61	111	77 original
2906	23 Homoserine	141 Lanosta-8,24-dien-3-beta-ol	61 -0.278	-0.346	18.076	0.447	80	61	70	71	74	98 original
2907	23 Homoserine	24 [725; 2-Ketooctanoic acid (2TMS)]	64 -0.308	-0.848	31.894	0.612	81	60	131	10	133	17 original
2908	23 Homoserine	102 [904; Galactose methoxyamine (5TMS)]	64 -0.311	-0.615	12.383	0.503	82	58	92	49	25	64 original
2909	23 Homoserine	29 Erythritol	64 -0.311	-0.849	12.138	0.625	83	59	132	9	23	7 original
2910	23 Homoserine	126 [559; Erythritol (4TMS)]	45 -0.311	-0.606	13.335	0.517	84	57	91	50	34	58 original
2911	23 Homoserine	120 [945; Uridine (3TMS)]	54 -0.312	-0.330	13.767	0.504	85	56	69	72	41	20 original
2912	23 Homoserine	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64 -0.316	-0.574	31.846	0.500	86	55	87	54	132	69 original
2913	23 Homoserine	101 [832; Dopamine (4TMS)]	64 -0.319	-0.597	17.239	0.450	87	54	90	51	68	93 original
2914	23 Homoserine	97 [756; beta-D-Methylglucopyranoside (4TMS)]	52 -0.323	-0.567	25.049	0.454	88	53	88	55	119	91 original
2915	23 Homoserine	87 [945; beta-D-Glucopyranose (5TMS)]	62 -0.325	-0.555	34.671	0.439	89	52	84	57	136	104 original
2916	23 Homoserine	127 [777; Fructose-6-phosphate methoxyamine (8TMS)]	39 -0.325	-0.654	10.687	0.401	90	51	95	45	15	121 original
2917	23 Homoserine	78 Mannose	62 -0.327	-0.673	18.627	0.484	91	50	99	42	81	78 original
2918	23 Homoserine	16 [944; 2-Methyl-1,3-butanediol (2TMS)]	64 -0.327	-0.850	19.547	0.622	92	49	133	8	88	9 duplicate
2919	23 Homoserine	17 [700; 2-methyl-1,2-propanediol (2TMS)]	64 -0.332	-0.770	19.922	0.551	93	48	114	27	92	43 duplicate
2920	23 Homoserine	41 [639; Proline (2TMS)]	64 -0.333	-0.524	14.947	0.480	94	47	79	62	53	80 original
2921	23 Homoserine	19 Alanine (BP) (3TMS)	64 -0.334	-0.566	14.945	0.459	95	46	85	56	52	89 duplicate
2922	23 Homoserine	39 [829; 1-Phenylethanol (1TMS)]	63 -0.339	-0.865	22.442	0.618	96	45	134	7	107	13 original
2923	23 Homoserine	11 Succinic acid	64 -0.345	-0.787	12.396	0.574	97	44	117	24	26	35 duplicate
2924	23 Homoserine	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45 -0.352	-0.664	14.011	0.425	98	43	97	44	45	110 original
2925	23 Homoserine	46 Arabinose	64 -0.354	-0.802	24.188	0.622	99	42	124	17	114	10 original
2926	23 Homoserine	35 Pyroglutamic acid	64 -0.357	-0.653	39.381	0.500	100	41	95	46	139	68 original
2927	23 Homoserine	86 [793; D-Galactono-1,4-lactone (4TMS)]	61 -0.358	-0.765	27.679	0.598	101	40	113	28	125	22 original
2928	23 Homoserine	54 [NA]	55 -0.359	-0.734	18.245	0.491	102	39	107	34	77	74 original

2883	23 Homoserine	57	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55	-0.362	-0.771	21,263	0.582	103	38	116	25	101	29 original
2884	23 Homoserine	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.364	-0.892	13,601	0.618	104	37	139	2	39	12 original
2882	23 Homoserine	56	[829; Orotic acid (3TMS)]	64	-0.368	-0.814	20,159	0.610	105	36	126	15	96	18 original
2955	23 Homoserine	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	-0.371	-0.805	20,166	0.543	106	35	125	16	97	46 original
2960	23 Homoserine	134	Isomaltose	64	-0.377	-0.837	26,531	0.622	107	34	129	12	126	11 original
2929	23 Homoserine	103	[648; Ethylamine (2TMS)]	63	-0.378	-0.705	21,151	0.511	108	33	104	37	89	59 original
2896	23 Homoserine	70	[683; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	-0.378	-0.505	18,775	0.409	109	32	78	63	83	117 original
2961	23 Homoserine	135	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	-0.383	-0.651	12,436	0.489	110	31	94	47	28	75 original
2911	23 Homoserine	85	[528; Methylcitric acid (4TMS)]	48	-0.383	-0.771	10,361	0.578	111	30	115	26	12	31 original
11439	23 Homoserine	12	Glyceric acid	63	-0.391	-0.835	16,398	0.585	112	29	128	13	61	27 duplicate
2938	23 Homoserine	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	-0.392	-0.708	19,583	0.507	113	27	105	36	89	62 original
2891	23 Homoserine	65	[846; 3-Deoxyglucitol (5TMS)]	63	-0.392	-0.832	22,901	0.618	114	28	127	14	110	14 original
2902	23 Homoserine	76	Fructose	64	-0.393	-0.701	27,081	0.525	115	25	103	38	123	53 original
2854	23 Homoserine	28	Malic acid	64	-0.393	-0.883	12,699	0.605	116	26	138	3	31	19 original
2866	23 Homoserine	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.395	-0.769	32,267	0.598	117	23	118	23	134	23 original
11694	23 Homoserine	14	Fumaric acid	64	-0.395	-0.872	14,937	0.629	118	24	137	4	51	6 duplicate
12192	23 Homoserine	18	[590; 1-Acetyl-2-thiohydantoin]	64	-0.396	-0.823	11,917	0.455	119	22	93	48	21	90 duplicate
2814	23 Homoserine	88	Gluconic acid	64	-0.398	-0.790	18,093	0.578	120	21	119	22	75	33 original
11567	23 Homoserine	13	Uracil	64	-0.401	-0.865	20,022	0.613	121	20	135	6	93	16 duplicate
2866	23 Homoserine	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	49	-0.405	-0.473	18,251	0.422	122	19	76	65	78	112 original
2941	23 Homoserine	115	Glucose-6-phosphate	62	-0.406	-0.679	24,944	0.531	123	18	100	41	118	52 original
2926	23 Homoserine	100	[857; Mannitol (6TMS)]	64	-0.406	-0.739	12,404	0.525	124	17	108	33	27	54 original
2876	23 Homoserine	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	-0.407	-0.839	22,808	0.589	125	16	130	11	109	28 original
2958	23 Homoserine	132	[895; Isomaltose methoxyamine (8TMS)]	42	-0.412	-0.868	20,087	0.503	126	15	136	5	95	65 original
2947	23 Homoserine	121	[657; Erythritol (4TMS)]	55	-0.414	-0.690	18,529	0.488	127	14	102	39	80	76 original
2900	23 Homoserine	74	[912; Tetradecanoic acid (1TMS)]	64	-0.415	-0.666	17,703	0.507	128	13	98	43	70	61 original
2888	23 Homoserine	62	[812; D-Xylofuranose (4TMS)]	64	-0.416	-0.757	15,154	0.578	129	12	110	31	55	32 original
2870	23 Homoserine	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	-0.420	-0.682	16,407	0.489	130	11	101	40	62	85 original
2918	23 Homoserine	92	[680; Glycerol-2-phosphate (4TMS)]	54	-0.421	-0.544	15,104	0.426	131	10	82	59	54	109 original
2943	23 Homoserine	117	[724; Glycerol (3TMS)]	56	-0.429	-0.764	16,279	0.522	132	9	112	29	60	55 original
2936	23 Homoserine	110	[715; Erythritol (4TMS)]	54	-0.430	-0.741	19,094	0.569	133	8	109	32	85	39 original
2942	23 Homoserine	116	[882; Pseudouridine (5TMS)]	30	-0.430	-0.547	13,382	0.355	134	7	83	58	36	133 original
2932	23 Homoserine	122	[844; Erythritol (4TMS)]	52	-0.440	-0.797	20,951	0.532	135	6	121	20	98	50 original
2931	23 Homoserine	105	[705; 2-Ketogluconic acid (5TMS)]	62	-0.443	-0.762	17,955	0.599	136	5	111	30	72	21 original
12555	23 Homoserine	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	48	-0.443	-0.714	18,275	0.452	137	4	106	35	79	92 original
2852	23 Homoserine	26	Citramalic acid	64	-0.443	-0.800	17,228	0.581	138	3	122	19	65	30 duplicate
12674	23 Homoserine	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	-0.450	-0.801	15,754	0.522	139	2	123	18	58	56 original
11946	24 [725; 2-Ketooctanoic acid]	16	[844; 2-Methyl-1,3-butanediol (2TMS)]	52	-0.511	-0.910	18,135	0.584	140	1	140	1	76	28 duplicate
3000	24 [725; 2-Ketooctanoic acid]	57	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	64	0.942	0.994	14,933	0.734	1	140	1	140	21	2 duplicate
2889	24 [725; 2-Ketooctanoic acid]	46	Arabinose	55	0.879	0.962	25,715	0.702	2	139	12	129	63	11 original
3008	24 [725; 2-Ketooctanoic acid]	65	[846; 3-Deoxyglucitol (5TMS)]	64	0.874	0.980	22,367	0.725	3	138	7	134	49	6 original
11568	24 [725; 2-Ketooctanoic acid]	29	Uracil	63	0.860	0.986	32,934	0.724	4	137	4	137	98	7 original
2972	24 [725; 2-Ketooctanoic acid]	13	Erythritol	64	0.845	0.989	17,600	0.734	5	136	2	139	30	3 duplicate
3072	24 [725; 2-Ketooctanoic acid]	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	64	0.842	0.971	30,557	0.653	6	135	10	131	85	31 original
3029	24 [725; 2-Ketooctanoic acid]	86	[793; D-Galactono-1,4-lactone (4TMS)]	59	0.838	0.975	29,729	0.690	7	134	9	132	82	14 original
				61	0.837	0.960	20,930	0.726	8	133	13	128	42	5 original

2999	24 [725; 2-Ketocitranilic acid 56	[829; Oxalic acid (3TMS)]	64	0.836	0.981	33.102	0.733	9	132	5	138	100	4 original
3077	24 [725; 2-Ketocitranilic acid 134	Isomaltose	64	0.835	0.988	12.002	0.738	10	131	3	138	13	1 original
12070	24 [725; 2-Ketocitranilic acid 17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	0.832	0.949	15.738	0.629	11	130	15	126	24	42 duplicate
2982	24 [725; 2-Ketocitranilic acid 39	[829; 1-Phenylethanol (1TMS)]	63	0.814	0.980	20.885	0.681	12	129	6	135	40	19 original
11311	24 [725; 2-Ketocitranilic acid 11	Succinic acid	64	0.798	0.929	26.407	0.614	13	128	20	121	65	53 duplicate
2993	24 [725; 2-Ketocitranilic acid 50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	0.797	0.963	45.568	0.658	14	127	11	130	137	28 original
2981	24 [725; 2-Ketocitranilic acid 38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.793	0.976	26.631	0.682	15	126	8	133	68	18 original
2997	24 [725; 2-Ketocitranilic acid 54	[NA]	55	0.782	0.938	35.941	0.618	16	125	16	125	110	50 original
3031	24 [725; 2-Ketocitranilic acid 88	Gluconic acid	64	0.763	0.932	23.761	0.706	17	124	18	123	55	10 original
3005	24 [725; 2-Ketocitranilic acid 62	[812; D-Xylofuranose (4TMS)]	64	0.733	0.917	18.958	0.652	18	123	22	119	36	33 original
11695	24 [725; 2-Ketocitranilic acid 14	Fumaric acid	64	0.700	0.936	35.815	0.633	19	122	17	124	109	39 duplicate
11440	24 [725; 2-Ketocitranilic acid 12	Glycamic acid	63	0.700	0.898	37.881	0.598	20	121	23	118	113	60 duplicate
3042	24 [725; 2-Ketocitranilic acid 99	[662; Ribose-5-phosphate methoxamine (BP) (5TMS)]	41	0.688	0.952	32.864	0.652	21	120	14	127	97	32 original
2971	24 [725; 2-Ketocitranilic acid 28	Malic acid	64	0.655	0.931	24.404	0.654	22	119	19	122	58	30 original
3048	24 [725; 2-Ketocitranilic acid 103	[648; Ethylamine (2TMS)]	63	0.645	0.849	26.316	0.608	23	118	30	111	64	56 original
3035	24 [725; 2-Ketocitranilic acid 92	[680; Glycero-2-phosphate (4TMS)]	54	0.637	0.785	29.908	0.611	24	117	41	100	83	55 original
12675	24 [725; 2-Ketocitranilic acid 22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.627	0.921	36.070	0.620	25	116	21	120	111	48 duplicate
3019	24 [725; 2-Ketocitranilic acid 76	Fructose	64	0.623	0.887	10.015	0.583	26	115	25	116	8	17 original
3016	24 [725; 2-Ketocitranilic acid 73	[708; Glucose methoxamine (5TMS)]	57	0.614	0.786	30.645	0.556	27	114	40	101	86	74 original
2983	24 [725; 2-Ketocitranilic acid 40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.605	0.858	7.259	0.615	28	113	29	112	2	51 original
3021	24 [725; 2-Ketocitranilic acid 78	Mannose	62	0.602	0.828	33.545	0.604	29	112	34	107	103	58 original
3048	24 [725; 2-Ketocitranilic acid 105	[705; 2-Ketogluconic acid (5TMS)]	48	0.587	0.873	24.990	0.658	30	111	26	115	61	27 original
3068	24 [725; 2-Ketocitranilic acid 125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	0.586	0.803	6.926	0.622	31	110	36	105	1	47 original
2978	24 [725; 2-Ketocitranilic acid 35	Pyroglutamic acid	64	0.581	0.860	10.896	0.649	32	109	28	113	11	35 original
3013	24 [725; 2-Ketocitranilic acid 70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	0.570	0.807	13.727	0.527	33	108	57	84	16	87 original
12556	24 [725; 2-Ketocitranilic acid 21	[676; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	0.566	0.788	16.613	0.570	34	107	39	102	27	69 duplicate
3040	24 [725; 2-Ketocitranilic acid 97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	0.564	0.803	18.849	0.591	35	106	37	104	35	64 original
3058	24 [725; 2-Ketocitranilic acid 115	Glucose-6-phosphate	62	0.557	0.844	8.532	0.661	36	105	32	109	3	26 original
3049	24 [725; 2-Ketocitranilic acid 106	[733; Threitol (4TMS)]	62	0.552	0.865	26.472	0.691	37	104	27	114	68	13 original
2969	24 [725; 2-Ketocitranilic acid 26	Citramalic acid	64	0.536	0.791	17.050	0.534	38	103	38	103	28	81 original
3044	24 [725; 2-Ketocitranilic acid 101	[832; Dopamine (4TMS)]	64	0.534	0.751	27.964	0.552	39	102	44	97	73	76 original
9966	24 [725; 2-Ketocitranilic acid 1	[938; Sulfuric acid (2TMS)]	36	0.524	0.657	28.542	0.601	40	101	56	85	75	59 duplicate
3063	24 [725; 2-Ketocitranilic acid 120	[945; Uridine (3TMS)]	54	0.508	0.383	21.167	0.667	41	100	69	72	43	23 original
3034	24 [725; 2-Ketocitranilic acid 91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	0.494	0.700	28.865	0.511	42	99	50	91	78	96 original
3071	24 [725; 2-Ketocitranilic acid 128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.493	0.846	24.789	0.633	43	98	31	110	60	38 original
3055	24 [725; 2-Ketocitranilic acid 112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.460	0.698	44.280	0.518	44	97	51	90	136	92 original
3043	24 [725; 2-Ketocitranilic acid 100	[857; Mannitol (6TMS)]	64	0.457	0.761	25.223	0.553	45	95	43	98	62	75 original
3045	24 [725; 2-Ketocitranilic acid 102	[904; Galactose methoxamine (5TMS)]	64	0.457	0.680	32.823	0.542	46	96	54	87	96	79 original
3064	24 [725; 2-Ketocitranilic acid 121	[657; Erythritol (4TMS)]	55	0.448	0.732	39.410	0.626	47	94	46	95	120	45 original
3030	24 [725; 2-Ketocitranilic acid 87	[945; beta-D-Glucopyranose (5TMS)]	62	0.446	0.730	9.187	0.545	48	93	47	94	5	78 original
3060	24 [725; 2-Ketocitranilic acid 117	[724; Glycerol (3TMS)]	56	0.445	0.775	30.971	0.597	49	92	42	98	89	61 original
10651	24 [725; 2-Ketocitranilic acid 6	Glycerol	64	0.441	0.707	12.023	0.578	50	91	49	92	14	68 duplicate
3053	24 [725; 2-Ketocitranilic acid 110	[715; Erythritol (4TMS)]	54	0.441	0.813	33.683	0.697	51	90	35	106	105	12 original
3065	24 [725; 2-Ketocitranilic acid 122	[644; Erythritol (4TMS)]	52	0.427	0.839	39.554	0.628	52	89	33	108	121	43 original
3078	24 [725; 2-Ketocitranilic acid	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	0.381	0.574	21.476	0.510	53	88	60	81	45	97 original
3075	24 [725; 2-Ketocitranilic acid 132	[895; Isomaltose methoxamine (8TMS)]	42	0.380	0.897	36.885	0.622	54	87	24	117	112	46 original
3028	24 [725; 2-Ketocitranilic acid 85	[529; Methylcitric acid (4TMS)]	48	0.371	0.690	23.816	0.477	55	86	52	89	54	109 original
3056	24 [725; 2-Ketocitranilic acid 113	Galactose-6-phosphate	62	0.357	0.723	33.343	0.588	56	85	48	93	102	65 original
12193	24 [725; 2-Ketocitranilic acid 18	[590; 1-Acetyl-2-thiohydantoin]	64	0.356	0.553	26.946	0.458	57	84	63	78	70	114 duplicate
2987	24 [725; 2-Ketocitranilic acid 44	[910; 2-Ketogluconic acid methoxamine (4TMS)]	50	0.353	0.749	26.838	0.640	58	83	45	96	69	36 original

3070	24 [725; 2-Ketooctanoic acid 127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.285	0.678	27.274	0.651	59	82	55	88	71	34 original
12315	24 [725; 2-Ketooctanoic acid 19 Alanine (BP) (3TMS)	64	0.275	0.598	22.756	0.558	60	81	59	82	51	73 duplicate
3017	24 [725; 2-Ketooctanoic acid 74 [912; Tetradecanoic acid (1TMS)]	64	0.268	0.563	32.507	0.520	61	80	61	80	94	91 original
3057	24 [725; 2-Ketooctanoic acid 114 Fructose-6-phosphate	53	0.267	0.684	33.117	0.605	62	79	53	88	101	57 original
3023	24 [725; 2-Ketooctanoic acid 80 [772; D-Glucose (5TMS)]	62	0.261	0.607	9.853	0.514	63	78	58	83	7	93 original
3069	24 [725; 2-Ketooctanoic acid 128 [539; Erythritol (4TMS)]	45	0.261	0.559	31.324	0.679	64	77	62	79	90	21 original
3047	24 [725; 2-Ketooctanoic acid 104 [795; Erythritol (4TMS)]	63	0.257	0.469	29.658	0.567	65	76	66	75	80	71 original
3059	24 [725; 2-Ketooctanoic acid 116 [892; Pseudouridine (5TMS)]	30	0.228	0.375	23.837	0.453	66	75	70	71	57	116 original
3039	24 [725; 2-Ketooctanoic acid 96 myo-Inositol	49	0.219	0.213	42.806	0.306	67	74	78	63	133	140 original
3027	24 [725; 2-Ketooctanoic acid 84 Mannitol	62	0.213	0.529	10.267	0.478	68	73	64	77	9	107 original
2984	24 [725; 2-Ketooctanoic acid 41 [639; Proline (2TMS)]	64	0.188	0.427	20.580	0.488	69	72	67	74	38	103 original
3026	24 [725; 2-Ketooctanoic acid 83 Sorbitol	58	0.183	-0.330	16.230	0.376	70	71	92	49	25	136 original
2990	24 [725; 2-Ketooctanoic acid 47 [NA]	64	0.180	0.220	30.930	0.466	71	70	77	64	88	111 original
3068	24 [725; 2-Ketooctanoic acid 123 [945; Galactofuranose-6-phosphate (7TMS)]	64	0.176	0.416	23.435	0.579	72	69	68	73	52	66 original
3036	24 [725; 2-Ketooctanoic acid 93 [607; Putrescine (4TMS)]	60	0.178	0.321	42.497	0.439	73	68	72	69	132	124 original
11821	24 [725; 2-Ketooctanoic acid 15 Alanine	64	0.141	0.300	17.127	0.677	74	67	73	68	29	22 duplicate
3007	24 [725; 2-Ketooctanoic acid 79 Glucose	63	0.120	0.236	31.514	0.449	75	66	75	66	91	118 original
3022	24 [725; 2-Ketooctanoic acid 111 [583; Erythritol (4TMS)]	64	0.096	0.521	8.546	0.631	76	65	65	76	4	41 original
3054	24 [725; 2-Ketooctanoic acid 53 Glycerol-2-phosphate	42	0.071	0.268	44.052	0.402	77	64	74	67	135	132 original
2996	24 [725; 2-Ketooctanoic acid 133 [855; Squalene]	64	0.035	-0.042	38.494	0.401	78	63	85	56	117	133 original
3076	24 [725; 2-Ketooctanoic acid 90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	64	0.031	-0.022	29.971	0.395	79	62	82	59	84	134 original
3033	24 [725; 2-Ketooctanoic acid 109 Octadecanoic acid	64	-0.003	-0.028	28.673	0.424	80	61	84	57	76	128 original
3052	24 [725; 2-Ketooctanoic acid 140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49	-0.019	0.323	18.129	0.526	81	60	71	70	31	88 original
3083	24 [725; 2-Ketooctanoic acid 63 Glutamine	52	-0.026	-0.700	37.690	0.717	83	58	115	26	114	8 original
3061	24 [725; 2-Ketooctanoic acid 118 [928; Glucopyranose-6-phosphate (6TMS)]	58	-0.064	0.148	33.621	0.445	84	57	80	61	104	122 original
3037	24 [725; 2-Ketooctanoic acid 94 Hexadecanoic acid	64	-0.065	0.224	15.417	0.529	85	56	76	65	23	85 original
3084	24 [725; 2-Ketooctanoic acid 141 Lanosta-8,24-dien-3-beta-ol	61	-0.114	0.040	40.102	0.522	86	55	81	60	124	90 original
3015	24 [725; 2-Ketooctanoic acid 72 [919; D-Xylopyranose (4TMS)]	63	-0.123	-0.180	34.362	0.346	87	54	88	53	108	138 original
3082	24 [725; 2-Ketooctanoic acid 139 [700; Ergosta-5,7-dien-3-ol]	38	-0.149	-0.204	39.876	0.441	88	53	89	52	122	123 original
3050	24 [725; 2-Ketooctanoic acid 107 9-(Z)-Octadecenoic acid	64	-0.152	-0.284	20.333	0.417	89	52	91	50	37	129 original
3081	24 [725; 2-Ketooctanoic acid 138 [697; Ergosterol (1TMS)]	46	-0.154	-0.025	40.079	0.478	90	51	83	58	123	108 original
3014	24 [725; 2-Ketooctanoic acid 71 [731; Erythrose (3TMS)]	64	-0.163	-0.269	22.272	0.479	91	50	90	51	48	106 original
3080	24 [725; 2-Ketooctanoic acid 137 Ergosterol	64	-0.167	-0.160	24.588	0.499	92	49	87	54	59	102 original
3062	24 [725; 2-Ketooctanoic acid 119 [931; myo-Inositol-2-phosphate (7TMS)]	64	-0.186	-0.154	29.365	0.552	93	48	86	55	79	77 original
2895	24 [725; 2-Ketooctanoic acid 52 [NA]	46	-0.186	-0.614	42.293	0.685	94	47	107	34	131	15 original
2866	24 [725; 2-Ketooctanoic acid 43 [548; Leucine (2TBS)]	60	-0.205	-0.422	27.707	0.509	95	46	95	48	72	98 original
2868	24 [725; 2-Ketooctanoic acid 25 [709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.227	-0.909	36.406	0.640	96	45	135	6	116	37 original
10380	24 [725; 2-Ketooctanoic acid 4 Phosphoric acid	51	-0.236	-0.459	11.598	0.328	97	44	97	44	12	139 duplicate
3067	24 [725; 2-Ketooctanoic acid 124 [734; 1-Monoleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]	59	-0.258	-0.379	50.644	0.426	98	43	93	48	140	127 original
3073	24 [725; 2-Ketooctanoic acid 130 Trehalose	63	-0.263	-0.381	9.600	0.381	99	42	94	47	6	135 original
3011	24 [725; 2-Ketooctanoic acid 68 [570; Hypoxanthine (2TMS)]	20	-0.263	-0.914	28.487	0.619	100	41	136	5	74	49 original
3004	24 [725; 2-Ketooctanoic acid 61 [NA]	64	-0.269	-0.446	30.713	0.500	101	40	98	45	87	101 original
3041	24 [725; 2-Ketooctanoic acid 98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	64	-0.280	-0.765	42.235	0.578	102	39	122	19	130	67 original
12793	24 [725; 2-Ketooctanoic acid 23 Homoserine	48	-0.308	-0.848	31.894	0.612	103	38	128	13	92	54 duplicate
3079	24 [725; 2-Ketooctanoic acid 136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.324	-0.472	18.183	0.447	104	37	98	43	32	121 original
3001	24 [725; 2-Ketooctanoic acid 58 [636; 4R-Acetamid-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	-0.329	-0.480	21.934	0.406	105	36	99	42	46	130 original
2970	24 [725; 2-Ketooctanoic acid 27 [815; (E)-4-Methyl-5-hydroxy-3-pentan-2-one (1TMS)]	53	-0.329	-0.836	41.202	0.584	106	35	126	15	126	72 original
10785	24 [725; 2-Ketooctanoic acid 7 Threonine	64	-0.333	-0.576	10.520	0.430	107	34	101	40	10	126 duplicate

3032	24 [725; 2-Ketocrotonic acid]	89	[775; Dopamine (4TMS)]	35	-0.345	-0.831	32.623	0.592	108	33	124	17	95	63 original
3051	24 [725; 2-Ketocrotonic acid]	108	Octadecanoic acid	64	-0.349	-0.519	34.250	0.404	109	32	100	41	107	131 original
3018	24 [725; 2-Ketocrotonic acid]	75	Lysine	64	-0.372	-0.591	14.802	0.468	110	31	104	37	20	112 original
2979	24 [725; 2-Ketocrotonic acid]	36	[596; N-Acetylglutamic acid (2TMS)]	64	-0.385	-0.612	13.885	0.448	111	30	108	35	18	120 original
3009	24 [725; 2-Ketocrotonic acid]	66	Glycine acid-3-phosphate	64	-0.388	-0.659	33.732	0.486	112	29	111	30	106	104 original
2988	24 [725; 2-Ketocrotonic acid]	45	Homocysteine	61	-0.390	-0.611	48.919	0.433	113	28	105	38	139	125 original
10105	24 [725; 2-Ketocrotonic acid]	2	Serine	62	-0.401	-0.662	26.544	0.452	114	27	112	29	67	117 duplicate
10918	24 [725; 2-Ketocrotonic acid]	8	Isoleucine	55	-0.414	-0.591	22.528	0.355	115	28	103	38	50	137 duplicate
2974	24 [725; 2-Ketocrotonic acid]	31	[622; Parabanic acid (2TMS)]	64	-0.443	-0.739	38.543	0.525	116	25	118	23	118	89 original
2992	24 [725; 2-Ketocrotonic acid]	49	[877; Pyrophosphoric acid (4TMS)]	64	-0.444	-0.590	47.470	0.483	117	24	102	39	138	105 original
2980	24 [725; 2-Ketocrotonic acid]	37	Phenylalanine	64	-0.464	-0.729	13.776	0.504	118	23	117	24	17	100 original
2977	24 [725; 2-Ketocrotonic acid]	34	Aspartic acid	64	-0.466	-0.658	14.494	0.513	119	22	110	31	19	94 original
3003	24 [725; 2-Ketocrotonic acid]	60	Glycerol-3-phosphate	64	-0.469	-0.636	15.414	0.531	120	21	108	33	22	83 original
3010	24 [725; 2-Ketocrotonic acid]	67	Citric acid	64	-0.481	-0.654	12.395	0.459	121	20	109	32	15	113 original
3038	24 [725; 2-Ketocrotonic acid]	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	-0.484	-0.673	42.933	0.569	122	19	113	28	134	70 original
2891	24 [725; 2-Ketocrotonic acid]	48	Asparagine	64	-0.487	-0.832	33.093	0.665	123	18	125	16	98	25 original
11050	24 [725; 2-Ketocrotonic acid]	9	Proline	63	-0.494	-0.706	23.820	0.449	124	17	116	25	56	119 duplicate
3074	24 [725; 2-Ketocrotonic acid]	131	[626; 5-Methylthioadenosine (3TMS)]	55	-0.512	-0.685	41.951	0.632	125	16	114	27	129	40 original
2976	24 [725; 2-Ketocrotonic acid]	33	Methionine	64	-0.517	-0.744	31.903	0.529	126	15	119	22	93	84 original
2988	24 [725; 2-Ketocrotonic acid]	55	[612; 4-Aminobutyric acid (2TBS)]	43	-0.546	-0.813	41.557	0.596	127	14	123	18	128	62 original
2994	24 [725; 2-Ketocrotonic acid]	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.550	-0.848	40.340	0.512	128	13	129	12	125	95 original
2983	24 [725; 2-Ketocrotonic acid]	30	[815; Ethyl-3(2H)-thiophenone]	64	-0.568	-0.750	18.212	0.457	129	12	120	21	33	115 original
10516	24 [725; 2-Ketocrotonic acid]	5	Leucine	45	-0.582	-0.861	28.827	0.540	130	11	132	9	77	80 duplicate
2975	24 [725; 2-Ketocrotonic acid]	32	[729; N,N-Dimethyllysine methyl ester]	63	-0.610	-0.878	41.483	0.626	131	10	133	8	127	44 original
10243	24 [725; 2-Ketocrotonic acid]	3	Ethanolamine	62	-0.627	-0.847	38.222	0.614	132	9	127	14	115	52 duplicate
3012	24 [725; 2-Ketocrotonic acid]	69	Arginine	60	-0.633	-0.927	22.221	0.655	133	8	137	4	47	29 original
3002	24 [725; 2-Ketocrotonic acid]	59	Ornithine; Arginine	64	-0.658	-0.766	16.287	0.532	134	7	121	20	26	82 original
11181	24 [725; 2-Ketocrotonic acid]	10	Glycine	64	-0.684	-0.955	21.428	0.713	135	6	139	2	44	9 duplicate
3020	24 [725; 2-Ketocrotonic acid]	77	[826; beta-[[[5-methyl-2-thienyl)methyl]eneamino-benzeneacetic acid methyl ester]	62	-0.684	-0.854	20.892	0.505	136	5	131	10	41	98 original
3024	24 [725; 2-Ketocrotonic acid]	81	Tyrosine	64	-0.712	-0.907	18.610	0.684	137	4	134	7	34	16 original
2885	24 [725; 2-Ketocrotonic acid]	42	Glutamic acid	60	-0.733	-0.850	23.534	0.528	138	3	130	11	53	86 original
3025	24 [725; 2-Ketocrotonic acid]	82	Lysine	39	-0.741	-0.973	20.675	0.667	139	2	140	1	39	24 original
12436	24 [725; 2-Ketocrotonic acid]	20	[619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.742	-0.933	29.683	0.681	140	1	138	3	81	20 duplicate
3190	25 [709; 2,5-Diaminovaleral	131	[626; 5-Methylthioadenosine (3TMS)]	41	0.822	0.622	13.188	0.519	1	140	24	117	22	65 original
3110	25 [709; 2,5-Diaminovaleral	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	29	0.586	0.815	16.047	0.494	2	139	9	132	45	80 original
3104	25 [709; 2,5-Diaminovaleral	45	Homocysteine	45	0.574	0.672	15.785	0.460	3	138	17	124	42	91 original
12794	25 [709; 2,5-Diaminovaleral	23	Homoserine	48	0.569	0.924	8.506	0.574	4	137	1	140	3	40 duplicate
10517	25 [709; 2,5-Diaminovaleral	5	Leucine	29	0.562	0.837	7.304	0.571	5	136	7	134	1	42 duplicate
3107	25 [709; 2,5-Diaminovaleral	48	Asparagine	48	0.560	0.789	9.168	0.608	6	135	12	129	6	27 original
12437	25 [709; 2,5-Diaminovaleral	20	[619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	17	0.559	0.785	14.728	0.530	7	134	13	128	32	58 duplicate
3127	25 [709; 2,5-Diaminovaleral	68	[570; Hypoxanthine (2TMS)]	10	0.556	0.924	8.707	0.213	8	133	2	139	5	140 original
3102	25 [709; 2,5-Diaminovaleral	43	[548; Leucine (2TBS)]	44	0.545	0.692	11.903	0.396	9	132	15	126	16	121 original
3157	25 [709; 2,5-Diaminovaleral	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	35	0.543	0.828	13.344	0.433	10	131	8	133	24	102 original
3128	25 [709; 2,5-Diaminovaleral	69	Arginine	44	0.522	0.891	16.631	0.616	11	130	5	136	50	23 original
10919	25 [709; 2,5-Diaminovaleral	8	Isoleucine	39	0.511	0.509	16.738	0.404	12	129	31	110	51	114 duplicate
3086	25 [709; 2,5-Diaminovaleral	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	37	0.502	0.899	10.768	0.526	13	128	3	138	10	64 original
3148	25 [709; 2,5-Diaminovaleral	89	[775; Dopamine (4TMS)]	19	0.485	0.651	9.260	0.404	14	127	19	122	7	116 original
3108	25 [709; 2,5-Diaminovaleral	49	[877; Pyrophosphoric acid (4TMS)]	48	0.482	0.479	15.047	0.455	15	126	35	106	34	94 original

3092	25	[709; 2,5-Diaminovalero	33	Methionine	48	0,479	0,658	11,124	0,400	16	125	18	123	13	118 original
3090	25	[709; 2,5-Diaminovalero	31	[622; Parabenic acid (2TMS)]	48	0,468	0,794	9,507	0,519	17	124	10	131	8	66 original
11182	25	[709; 2,5-Diaminovalero	10	Glycine	48	0,450	0,898	18,204	0,633	18	122	4	137	65	11 Juplicate
3089	25	[709; 2,5-Diaminovalero	30	[815; Ethyl-3(2H)-thiophenone]	48	0,450	0,841	27,923	0,364	19	123	20	121	114	133 original
3101	25	[709; 2,5-Diaminovalero	42	Glutamic acid	44	0,431	0,707	23,339	0,416	20	121	14	127	97	109 original
3093	25	[709; 2,5-Diaminovalero	34	Aspartic acid	48	0,420	0,600	32,154	0,395	21	120	25	116	128	123 original
3141	25	[709; 2,5-Diaminovalero	82	Lysine	23	0,415	0,883	7,660	0,623	22	119	6	135	2	16 original
11051	25	[709; 2,5-Diaminovalero	9	Proline	47	0,406	0,595	24,182	0,427	23	118	26	115	101	107 Juplicate
3118	25	[709; 2,5-Diaminovalero	59	Ornithine; Arginine	48	0,372	0,633	39,350	0,464	24	117	22	119	137	90 original
3114	25	[709; 2,5-Diaminovalero	55	[612; 4-Aminobutyric acid (2TBS)]	28	0,349	0,484	20,916	0,472	25	116	33	108	86	87 original
3091	25	[709; 2,5-Diaminovalero	32	[729; N,N-Dimethyllysine methyl ester] [626; beta-[(5-methyl-2-thienyl)methyl]eneamino-	47	0,343	0,792	8,592	0,583	26	115	11	130	4	36 original
3136	25	[709; 2,5-Diaminovalero		benzeneacetic acid methyl ester]											
10106	25	[709; 2,5-Diaminovalero	2	Serine	46	0,339	0,638	25,251	0,434	27	114	21	120	107	101 original
3122	25	[709; 2,5-Diaminovalero	63	Glutamine	46	0,329	0,576	17,445	0,385	28	113	27	114	59	124 Juplicate
3125	25	[709; 2,5-Diaminovalero	66	Glycetic acid-3-phosphate	38	0,317	0,184	11,810	0,578	29	112	48	92	15	38 original
3140	25	[709; 2,5-Diaminovalero	81	Tyrosine	48	0,309	0,632	11,451	0,513	30	111	23	118	14	73 original
3154	25	[709; 2,5-Diaminovalero	95	[770; 3,4,6-Trisidroxiphenylethanolamine (5TMS)]	48	0,307	0,677	30,283	0,595	31	110	16	125	119	31 original
3120	25	[709; 2,5-Diaminovalero	61	[NA]	34	0,273	0,365	17,621	0,275	32	109	38	103	61	139 original
10244	25	[709; 2,5-Diaminovalero	3	Ethanolamine	48	0,257	0,200	13,574	0,436	33	108	47	94	28	89 original
3134	25	[709; 2,5-Diaminovalero	75	Lysine	46	0,229	0,571	10,968	0,475	34	107	28	113	12	95 Juplicate
3096	25	[709; 2,5-Diaminovalero	37	Phenylalanine	48	0,216	0,532	39,198	0,427	35	105	29	112	136	106 original
			58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hidroxycyclohexane (1TMS)]	48	0,216	0,517	25,661	0,432	36	106	30	111	108	103 original
3117	25	[709; 2,5-Diaminovalero		(1TMS)]											
10786	25	[709; 2,5-Diaminovalero	7	Threonine	48	0,207	0,485	19,252	0,363	37	103	32	109	74	126 original
	25	[709; 2,5-Diaminovalero		Alanine	48	0,207	0,480	31,783	0,325	38	104	34	107	124	138 Juplicate
3095	25	[709; 2,5-Diaminovalero	38	[596; N-Acetylglutamic acid (2TMS)]	48	0,193	0,426	23,815	0,596	39	102	37	104	99	34 Juplicate
9987	25	[709; 2,5-Diaminovalero	1	[938; Sulfuric acid (2TMS)]	48	0,151	0,456	29,448	0,399	40	101	36	105	118	119 original
10381	25	[709; 2,5-Diaminovalero	4	Phosphoric acid	35	0,150	-0,425	15,768	0,541						

3183	25 [709; 2,5-Diaminovalero	124 [734; 1-Monocleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]	43 -0.189	-0.066	17.189	0.403	65	76	56	85	55	117 original
3166	25 [709; 2,5-Diaminovalero	107 9-(Z)-Octadecenol (1TMS)]	48 -0.191	-0.249	20.305	0.372	66	74	64	77	78	129 original
3163	25 [709; 2,5-Diaminovalero	104 [795; Erythritol (4TMS)]	47 -0.191	-0.253	16.540	0.470	67	75	65	78	49	88 original
3182	25 [709; 2,5-Diaminovalero	123 [945; Galactofuranose-6-phosphate (7TMS)]	48 -0.189	-0.087	18.718	0.485	68	73	57	84	71	82 original
12071	25 [709; 2,5-Diaminovalero	87 [945; beta-D-Glucopyranose (5TMS)]	46 -0.208	-0.533	40.833	0.577	69	72	83	58	138	39 original
3170	25 [709; 2,5-Diaminovalero	17 [700; 2-methyl-1,2-propanediol (2TMS)]	48 -0.216	-0.802	26.838	0.571	70	71	114	27	112	41 duplicate
3142	25 [709; 2,5-Diaminovalero	83 Sorbitol	36 -0.225	-0.226	14.187	0.366	71	70	62	79	30	132 original
11947	25 [709; 2,5-Diaminovalero	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	42 -0.226	0.187	22.606	0.414	72	69	48	93	83	112 original
12911	25 [709; 2,5-Diaminovalero	24 [725; 2-Ketocetonic acid (2TMS)]	48 -0.227	-0.890	26.688	0.621	73	67	128	13	110	19 duplicate
11569	25 [709; 2,5-Diaminovalero	13 Urecl	48 -0.227	-0.909	38.406	0.640	74	68	135	6	134	9 duplicate
3164	25 [709; 2,5-Diaminovalero	105 [705; 2-Ketogluconic acid (5TMS)]	45 -0.232	-0.900	26.718	0.628	75	66	133	8	111	12 duplicate
		57	45 -0.238	-0.721	23.857	0.517	76	65	103	38	100	69 original
3116	25 [709; 2,5-Diaminovalero	[757; 2-Desoxy-pentose-3-yose dimethoxamine (2TMS)]	47 -0.241	-0.880	25.233	0.664	77	64	126	15	106	1 original
3187	25 [709; 2,5-Diaminovalero	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	42 -0.245	-0.714	19.617	0.529	78	63	99	42	76	60 original
3155	25 [709; 2,5-Diaminovalero	96 myo-inositol	33 -0.250	-0.122	13.230	0.369	79	62	59	82	23	130 original
3105	25 [709; 2,5-Diaminovalero	46 Arabinose	48 -0.257	-0.891	28.544	0.655	80	61	129	12	117	4 original
3098	25 [709; 2,5-Diaminovalero	39 [829; 1-Phenylethanol (1TMS)]	48 -0.261	-0.913	28.131	0.623	81	60	139	2	115	17 original
3192	25 [709; 2,5-Diaminovalero	133 [855; Squalene]	48 -0.262	-0.117	16.050	0.336	82	59	58	83	46	136 original
3124	25 [709; 2,5-Diaminovalero	65 [646; 3-Deoxyglucitol (5TMS)]	48 -0.266	-0.909	23.234	0.656	83	58	136	5	96	3 original
3088	25 [709; 2,5-Diaminovalero	29 Erythritol	48 -0.270	-0.877	16.006	0.652	84	57	125	16	44	6 original
3196	25 [709; 2,5-Diaminovalero	137 Ergosterol	48 -0.282	-0.156	20.436	0.423	85	56	60	81	81	108 original
3162	25 [709; 2,5-Diaminovalero	103 [648; Ethylamine (2TMS)]	48 -0.284	-0.634	25.171	0.479	86	54	92	49	105	83 original
3193	25 [709; 2,5-Diaminovalero	134 Isomaltose	48 -0.284	-0.904	35.228	0.658	87	55	134	7	129	2 original
3151	25 [709; 2,5-Diaminovalero	92 [680; Glycerol-2-phosphate (4TMS)]	46 -0.287	-0.586	17.408	0.527	88	53	89	52	57	63 original
11441	25 [709; 2,5-Diaminovalero	12 Glycetic acid	48 -0.293	-0.884	15.762	0.591	89	52	122	19	40	32 duplicate
3113	25 [709; 2,5-Diaminovalero	54 [NA]	47 -0.297	-0.815	18.695	0.581	90	51	117	24	70	37 original
3178	25 [709; 2,5-Diaminovalero	120 [945; Uridine (3TMS)]	45 -0.297	-0.226	20.350	0.812	91	50	61	80	80	25 original
		129 [940; Maltose methoxamine (6TMS); alpha-D-Glc-(1,4)-D-Glc]										
3188	25 [709; 2,5-Diaminovalero	50 [746; Ribonic acid-1,4-lactone (3TMS)]	48 -0.303	-0.870	23.000	0.823	92	47	124	17	95	18 original
3109	25 [709; 2,5-Diaminovalero	56 [829; Orolic acid (3TMS)]	48 -0.303	-0.895	20.558	0.841	94	49	131	10	83	15 original
3115	25 [709; 2,5-Diaminovalero	139 [700; Ergosterol-5,7-dien-3-ol]	27 -0.305	-0.337	10.910	0.374	95	46	69	72	11	128 original
3147	25 [709; 2,5-Diaminovalero	88 Gluconic acid	48 -0.307	-0.812	23.473	0.825	96	45	116	25	98	14 original
3188	25 [709; 2,5-Diaminovalero	127 [777; Fructose-6-phosphate methoxamine (6TMS)]	36 -0.311	-0.740	15.418	0.543	97	44	104	37	37	54 original
12316	25 [709; 2,5-Diaminovalero	19 Alanine (BP) (3TMS)	48 -0.324	-0.442	21.043	0.497	98	43	75	68	87	77 duplicate
11312	25 [709; 2,5-Diaminovalero	11 Succinic acid	48 -0.328	-0.817	18.016	0.602	99	42	118	23	63	28 duplicate
3172	25 [709; 2,5-Diaminovalero	113 Galactose-6-phosphate	47 -0.328	-0.479	15.897	0.532	100	41	80	61	43	57 original
3129	25 [709; 2,5-Diaminovalero	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	41 -0.332	-0.324	24.857	0.515	101	40	68	73	104	72 original
3178	25 [709; 2,5-Diaminovalero	119 [931; myo-Inositol-2-phosphate (7TMS)]	48 -0.335	-0.499	16.925	0.435	102	39	82	59	53	100 original
3100	25 [709; 2,5-Diaminovalero	41 [639; Proline (2TMS)]	48 -0.337	-0.381	21.660	0.437	103	38	71	70	90	96 original
3087	25 [709; 2,5-Diaminovalero	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	48 -0.342	-0.930	18.880	0.638	104	37	140	1	72	10 original
3197	25 [709; 2,5-Diaminovalero	138 [674; Ergosterol (1TMS)]	33 -0.352	-0.240	11.936	0.427	105	38	63	78	17	105 original
3145	25 [709; 2,5-Diaminovalero	86 [793; D-Galactono-1,4-lactone (4TMS)]	45 -0.354	-0.865	31.608	0.621	106	35	123	18	123	20 original
3168	25 [709; 2,5-Diaminovalero	109 Octadecanoic acid	48 -0.360	-0.470	30.293	0.449	107	34	77	64	120	95 original
3173	25 [709; 2,5-Diaminovalero	114 Fructose-6-phosphate	42 -0.366	-0.477	15.019	0.564	108	33	79	62	33	44 original
3184	25 [709; 2,5-Diaminovalero	125 [892; Sucrose (6TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	48 -0.376	-0.543	38.323	0.529	109	32	84	57	133	59 original
3153	25 [709; 2,5-Diaminovalero	94 Hexadecanoic acid	48 -0.387	-0.465	28.243	0.456	110	31	76	65	116	93 original
3144	25 [709; 2,5-Diaminovalero	85 [529; Methylcitric acid (4TMS)]	32 -0.395	-0.775	12.712	0.568	111	30	108	33	19	43 original
3132	25 [709; 2,5-Diaminovalero	73 [708; Glucose methoxamine (5TMS)]	41 -0.402	-0.620	17.758	0.518	112	29	90	51	62	68 original

3137	25 [709; 2,5-Diaminovalero	78	Mannose	46	-0.405	-0.688	18.601	0.552	113	28	97	44	67	49	original
3200	25 [709; 2,5-Diaminovalero	141	Lanosta-8,24-dien-3- $\beta$ -ol	45	-0.410	-0.554	16.902	0.516	114	27	86	55	52	71	original
11696	25 [709; 2,5-Diaminovalero	14	Fumaric acid	48	-0.422	-0.894	15.453	0.612	115	26	130	11	38	24	duplicate
3194	25 [709; 2,5-Diaminovalero		[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (6TMS)]	48	-0.429	-0.666	19.652	0.432	116	25	94	47	77	104	original
3121	25 [709; 2,5-Diaminovalero	62	[812; D-Xylofuranose (4TMS)]	48	-0.440	-0.834	22.359	0.620	117	24	120	21	92	21	original
3199	25 [709; 2,5-Diaminovalero	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	33	-0.455	-0.624	13.192	0.494	118	23	91	50	21	79	original
3171	25 [709; 2,5-Diaminovalero	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	47	-0.458	-0.718	15.067	0.475	119	22	102	39	35	86	original
12184	25 [709; 2,5-Diaminovalero	18	[590; 1-Acetyl-2-thiohydantoin]	48	-0.463	-0.580	17.500	0.475	120	21	88	53	60	84	duplicate
12557	25 [709; 2,5-Diaminovalero	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	48	-0.473	-0.775	24.345	0.527	121	20	109	32	102	62	duplicate
3085	25 [709; 2,5-Diaminovalero	26	Citramalic acid	48	-0.484	-0.761	22.911	0.519	122	19	108	35	94	67	original
12676	25 [709; 2,5-Diaminovalero	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	42	-0.491	-0.911	17.416	0.598	123	18	138	3	58	29	duplicate
3087	25 [709; 2,5-Diaminovalero	28	Malic acid	48	-0.512	-0.900	19.106	0.551	124	17	132	9	73	51	original
3191	25 [709; 2,5-Diaminovalero	132	[895; Isomaltose methoxyamine (8TMS)]	38	-0.514	-0.909	20.489	0.564	125	16	137	4	82	45	original
3175	25 [709; 2,5-Diaminovalero	116	[692; Pseudouridine (5TMS)]	20	-0.516	-0.824	13.472	0.538	126	15	85	56	26	56	original
3133	25 [709; 2,5-Diaminovalero	74	[912; Tetradecanoic acid (1TMS)]	48	-0.523	-0.860	20.671	0.459	127	14	93	48	84	92	original
3099	25 [709; 2,5-Diaminovalero	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	48	-0.534	-0.811	37.253	0.588	128	13	115	26	132	35	original
3103	25 [709; 2,5-Diaminovalero	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	45	-0.541	-0.743	21.079	0.598	129	12	105	36	89	30	original
3161	25 [709; 2,5-Diaminovalero	102	[904; Galactose methoxyamine (5TMS)]	45	-0.543	-0.717	16.222	0.509	130	11	100	41	36	76	original
3169	25 [709; 2,5-Diaminovalero	110	[715; Erythritol (4TMS)]	46	-0.552	-0.791	20.306	0.653	131	10	112	29	79	5	original
3180	25 [709; 2,5-Diaminovalero	121	[657; Erythritol (4TMS)]	44	-0.552	-0.685	16.186	0.529	132	9	85	46	47	61	original
3176	25 [709; 2,5-Diaminovalero	117	[724; Glycerol (3TMS)]	45	-0.564	-0.790	19.284	0.548	133	8	107	34	128	52	original
3135	25 [709; 2,5-Diaminovalero	76	Fructose	48	-0.566	-0.774	33.783	0.548	134	6	107	34	128	52	original
3159	25 [709; 2,5-Diaminovalero	100	[857; Mannitol (6TMS)]	48	-0.568	-0.780	18.673	0.556	135	7	111	30	69	48	original
3094	25 [709; 2,5-Diaminovalero	35	Pyrogulamic acid	48	-0.569	-0.717	44.229	0.516	136	5	101	40	140	70	original
3174	25 [709; 2,5-Diaminovalero	115	Glucose-6-phosphate	47	-0.576	-0.712	31.798	0.608	137	4	98	43	125	26	original
3185	25 [709; 2,5-Diaminovalero	126	[559; Erythritol (4TMS)]	42	-0.589	-0.867	17.329	0.618	138	3	96	45	56	22	original
3181	25 [709; 2,5-Diaminovalero	122	[644; Erythritol (4TMS)]	46	-0.592	-0.863	20.718	0.586	139	2	121	20	85	33	original
3165	25 [709; 2,5-Diaminovalero	106	[733; Threitol (4TMS)]	46	-0.596	-0.796	22.096	0.640	140	1	113	28	91	8	original
11697	26 Citramalic acid	14	Fumaric acid	64	0.677	0.874	19.951	0.595	1	140	1	140	97	2	duplicate
3202	26 Citramalic acid	28	Malic acid	64	0.637	0.863	8.452	0.612	2	139	3	138	19	1	original
12677	26 Citramalic acid	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.626	0.867	21.978	0.562	3	138	2	139	108	6	duplicate
11313	26 Citramalic acid	11	Succinic acid	64	0.621	0.835	10.593	0.553	4	137	4	137	27	9	duplicate
12558	26 Citramalic acid	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	0.600	0.831	2.896	0.534	5	136	5	136	1	24	duplicate
3289	26 Citramalic acid	115	Glucose-6-phosphate	62	0.575	0.714	10.287	0.506	6	135	35	106	25	48	original
3214	26 Citramalic acid	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.573	0.813	18.880	0.526	7	134	7	134	91	30	original
11442	26 Citramalic acid	12	Glyceric acid	63	0.557	0.807	22.145	0.554	8	133	8	133	109	7	duplicate
12195	26 Citramalic acid	18	[590; 1-Acetyl-2-thiohydantoin]	64	0.555	0.753	10.753	0.466	9	132	24	117	28	69	duplicate
3280	26 Citramalic acid	106	[733; Threitol (4TMS)]	62	0.552	0.767	13.567	0.572	10	131	19	122	45	4	original
3306	26 Citramalic acid	132	[895; Isomaltose methoxyamine (8TMS)]	42	0.547	0.798	23.519	0.526	11	130	11	130	114	31	original
3209	26 Citramalic acid	35	Pyrogulamic acid	64	0.544	0.714	25.878	0.472	12	129	34	107	122	65	original
11048	26 Citramalic acid	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	0.542	0.793	5.267	0.547	13	128	13	128	5	15	duplicate
3203	26 Citramalic acid	29	Erythritol	64	0.539	0.807	14.566	0.545	14	127	9	132	52	16	original
12912	26 Citramalic acid	24	[725; 2-Ketoclanonic acid (2TMS)]	64	0.536	0.791	17.050	0.534	15	126	14	127	71	23	duplicate
3212	26 Citramalic acid	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.535	0.824	11.260	0.549	16	125	6	135	30	14	original
3236	26 Citramalic acid	62	[812; D-Xylofuranose (4TMS)]	64	0.533	0.744	3.791	0.539	17	124	27	114	2	19	original
3250	26 Citramalic acid	76	Fructose	64	0.530	0.735	12.808	0.534	18	123	30	111	38	26	original
12317	26 Citramalic acid	19	Alanine (BP) (3TMS)	64	0.527	0.704	8.114	0.488	19	122	37	104	17	58	duplicate
3260	26 Citramalic acid	86	[793; D-Galactono-1,4-lactone (4TMS)]	61	0.527	0.779	17.890	0.550	20	121	15	126	80	13	original
3290	26 Citramalic acid	116	[882; Pseudouridine (5TMS)]	30	0.526	0.600	14.468	0.316	21	120	51	90	50	139	original
3284	26 Citramalic acid	110	[715; Erythritol (4TMS)]	54	0.525	0.757	19.761	0.551	22	119	21	120	93	11	original



3295	26 Citramalic acid	121 [657; Erythritol (4TMS)]	55 0.521	0.723	24,135	0.520	23	118	33	108	115	38 original
11570	26 Citramalic acid	13 Uracil	64 0.520	0.793	7,840	0.571	24	117	12	128	15	5 duplicate
3291	26 Citramalic acid	117 [724; Glycerol (3TMS)]	56 0.514	0.752	18,400	0.522	25	116	25	116	67	33 original
3213	26 Citramalic acid	39 [829; 1-Phenylethanol (1TMS)]	63 0.512	0.799	12,343	0.551	26	115	10	131	34	12 original
3230	26 Citramalic acid	56 [829; Orotic acid (3TMS)]	64 0.505	0.764	19,853	0.527	27	114	20	121	95	29 original
3296	26 Citramalic acid	122 [644; Erythritol (4TMS)]	52 0.501	0.756	24,956	0.575	28	113	23	118	118	3 original
3299	26 Citramalic acid	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64 0.499	0.698	17,809	0.461	29	112	46	95	78	75 original
3215	26 Citramalic acid	41 [839; Proline (2TMS)]	64 0.494	0.698	5,386	0.498	30	111	42	99	6	51 original
3252	26 Citramalic acid	78 Mannose	62 0.490	0.704	19,859	0.483	31	110	38	103	96	61 original
12072	26 Citramalic acid	17 [700; 2-methyl-1,2-propanediol (2TMS)]	64 0.481	0.731	6,756	0.461	32	109	31	110	9	76 duplicate
3274	26 Citramalic acid	100 [857; Mannitol (6TMS)]	64 0.475	0.642	9,332	0.486	33	108	45	96	22	59 original
3247	26 Citramalic acid	73 [708; Glucose methoxyamine (5TMS)]	57 0.472	0.693	18,362	0.459	34	107	39	102	87	77 original
3239	26 Citramalic acid	65 [646; 3-Deoxyglucitol (5TMS)]	63 0.472	0.771	20,981	0.535	35	106	17	124	102	21 original
3224	26 Citramalic acid	50 [746; Ribonic acid-1,4-lactone (3TMS)]	61 0.470	0.750	30,058	0.495	36	105	26	115	136	53 original
3286	26 Citramalic acid	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63 0.470	0.707	28,156	0.468	37	104	36	105	130	88 original
3220	26 Citramalic acid	46 Arabinose	64 0.469	0.757	15,043	0.525	38	103	22	119	59	32 original
3262	26 Citramalic acid	88 Gluconic acid	64 0.465	0.727	11,433	0.517	39	102	32	109	31	41 original
3228	26 Citramalic acid	54 [NA]	55 0.464	0.661	21,605	0.495	40	101	43	98	104	54 original
3294	26 Citramalic acid	120 [945; Uridine (3TMS)]	54 0.462	0.426	6,365	0.554	41	100	67	74	8	8 original
3303	26 Citramalic acid	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59 0.461	0.768	17,247	0.519	42	99	18	123	74	40 original
3276	26 Citramalic acid	102 [904; Galactose methoxyamine (5TMS)]	64 0.459	0.595	16,727	0.494	43	98	52	89	69	55 original
3308	26 Citramalic acid	134 Isomaltose	64 0.456	0.773	14,315	0.538	44	97	16	125	48	20 original
3288	26 Citramalic acid	114 Fructose-6-phosphate	53 0.456	0.631	18,245	0.456	45	96	47	94	82	78 original
3248	26 Citramalic acid	74 [912; Tetradecanoic acid (1TMS)]	64 0.454	0.743	17,847	0.472	46	95	28	113	79	66 original
3309	26 Citramalic acid	135	64 0.452	0.690	4,737	0.472	47	94	41	100	4	67 original
3218	26 Citramalic acid	44 [902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	50 0.450	0.660	13,296	0.534	48	93	44	97	43	27 original
3244	26 Citramalic acid	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57 0.440	0.454	6,977	0.449	49	92	63	78	10	80 original
3300	26 Citramalic acid	126 [559; Erythritol (4TMS)]	45 0.428	0.627	15,988	0.515	50	91	49	92	66	43 original
3287	26 Citramalic acid	113 Galactose-6-phosphate	62 0.419	0.617	18,329	0.435	51	90	50	91	84	89 original
3231	26 Citramalic acid	57	55 0.411	0.692	15,313	0.522	52	89	40	101	61	34 original
3277	26 Citramalic acid	103 [757; 2-Desoxy-pentose-3-ylose dimethoxyamine (2TMS)]	63 0.401	0.568	15,741	0.500	53	88	54	87	63	49 original
3259	26 Citramalic acid	85 [529; Methylcitric acid (4TMS)]	48 0.388	0.736	11,968	0.514	54	87	29	112	32	44 original
3266	26 Citramalic acid	92 [680; Glycerol-2-phosphate (4TMS)]	54 0.370	0.507	15,700	0.435	55	86	58	83	62	90 original
3275	26 Citramalic acid	101 [832; Dopamine (4TMS)]	64 0.381	0.458	14,871	0.429	56	85	62	79	56	93 original
3261	26 Citramalic acid	87 [945; beta-D-Glucopyranose (5TMS)]	62 0.350	0.563	21,371	0.462	57	84	55	86	103	74 original
3270	26 Citramalic acid	96 myo-Inositol	49 0.349	0.353	29,351	0.351	58	83	73	68	134	134 original
3301	26 Citramalic acid	127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	39 0.347	0.537	12,052	0.493	59	82	57	84	33	56 original
3297	26 Citramalic acid	123 [945; Galactofuranose-6-phosphate (7TMS)]	64 0.338	0.451	7,519	0.448	60	81	64	77	13	82 original
10653	26 Citramalic acid	6 Glycerol	64 0.316	0.426	26,399	0.401	61	80	61	80	124	114 duplicate
3278	26 Citramalic acid	104 [795; Erythritol (4TMS)]	63 0.308	0.427	14,542	0.394	62	79	66	75	51	119 original
3302	26 Citramalic acid	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45 0.305	0.575	10,763	0.492	63	78	53	88	29	57 original
3285	26 Citramalic acid	111 [583; Erythritol (4TMS)]	42 0.289	0.407	29,436	0.452	64	77	68	73	135	79 original
3279	26 Citramalic acid	105 [705; 2-Ketogluconic acid (5TMS)]	48 0.278	0.481	13,055	0.508	65	76	60	81	39	46 original
3257	26 Citramalic acid	83 Sorbitol	58 0.251	-0.137	9,659	0.355	66	75	93	48	24	133 original
3265	26 Citramalic acid	91 [766; beta-D-Methylglucopyranoside (4TMS)]	64 0.250	0.376	19,276	0.412	67	74	71	70	92	101 original
3314	26 Citramalic acid	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49 0.243	0.372	25,557	0.394	68	73	72	69	120	118 original
3283	26 Citramalic acid	109 Octadecanoic acid	64 0.239	0.568	12,397	0.413	69	72	56	85	37	100 original
3271	26 Citramalic acid	97 [756; beta-D-Methylglucopyranoside (4TMS)]	52 0.232	0.398	14,897	0.422	70	71	69	72	57	97 original

3254	26 Citramalic acid	80	[772; D-Glucose (5TMS)]	52	0.231	0.444	17.327	0.405	71	70	65	76	75	111 original
3307	26 Citramalic acid	133	[655; Squalene]	64	0.223	0.241	13.846	0.365	72	69	76	65	46	130 original
3268	26 Citramalic acid	94	Hexadecanoic acid	64	0.212	0.503	8.836	0.411	73	68	59	82	21	103 original
3273	26 Citramalic acid	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	0.210	0.629	18.872	0.485	74	67	48	93	90	60 original
3238	26 Citramalic acid	64	[789; Tyramine (3TMS)]	63	0.198	0.182	15.074	0.401	75	66	79	62	60	113 original
11823	26 Citramalic acid	15	Alanine	64	0.177	0.202	7.185	0.517	76	65	78	63	12	42 duplicate
3312	26 Citramalic acid	138	[674; Ergosterol (1TMS)]	46	0.173	0.280	25.775	0.405	77	64	75	68	121	110 original
3253	26 Citramalic acid	79	Glucose	64	0.152	0.394	20.081	0.445	78	63	70	71	99	83 original
3313	26 Citramalic acid	139	[700; Ergosta-5,7-dien-3-ol]	38	0.127	0.028	26.927	0.316	79	62	88	53	125	140 original
3315	26 Citramalic acid	141	Lanosta-8,24-dien-3-beta-ol	61	0.113	0.228	24.725	0.395	80	61	77	64	117	117 original
3258	26 Citramalic acid	84	Mannitol	62	0.105	0.318	18.267	0.400	81	60	74	67	83	115 original
3292	26 Citramalic acid	118	[928; Glucopyranose-6-phosphate (6TMS)]	58	0.103	0.180	17.966	0.348	82	59	80	61	81	138 original
3311	26 Citramalic acid	137	Ergosterol	64	0.077	0.131	10.428	0.370	83	58	82	59	26	128 original
3245	26 Citramalic acid	71	[731; Erythrose (3TMS)]	64	0.065	0.053	5.500	0.410	84	57	85	56	7	105 original
3310	26 Citramalic acid	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.044	-0.100	8.058	0.417	85	56	91	50	16	99 original
3221	26 Citramalic acid	47	[NA]	64	0.037	0.033	16.545	0.406	86	55	87	54	68	108 original
3264	26 Citramalic acid	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	64	0.033	0.060	12.354	0.341	87	54	84	57	35	137 original
9868	26 Citramalic acid	1	[938; Sulfuric acid (2TMS)]	36	0.025	0.169	14.651	0.477	88	53	81	60	53	64 duplicate
3293	26 Citramalic acid	119	[931; myo-Inositol-2-phosphate (7TMS)]	64	0.019	0.090	13.171	0.411	89	52	83	58	41	104 original
3267	26 Citramalic acid	93	[607; Putrescine (4TMS)]	60	0.005	0.050	27.327	0.364	90	51	86	55	127	131 original
		124	[734; 1-Monoleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]	59	-0.019	-0.132	34.830	0.349	91	50	92	49	140	135 original
3298	26 Citramalic acid	107	9-(Z)-Octadecenoic acid	64	-0.023	-0.053	4.658	0.404	92	49	89	52	3	112 original
3281	26 Citramalic acid	72	[919; D-Xylopyranose (4TMS)]	63	-0.062	-0.095	18.543	0.372	93	48	90	51	88	127 original
3246	26 Citramalic acid	53	Glycerol-2-phosphate	64	-0.082	-0.155	22.162	0.327	94	47	94	47	110	138 original
3227	26 Citramalic acid	130	Trehalose	63	-0.123	-0.232	14.697	0.376	95	46	95	46	54	125 original
3304	26 Citramalic acid	4	Phosphoric acid	51	-0.150	-0.276	19.792	0.356	96	45	99	42	94	132 duplicate
10382	26 Citramalic acid	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	-0.151	-0.268	8.297	0.383	97	44	98	43	18	123 original
3232	26 Citramalic acid	7	Threonine	64	-0.167	-0.245	14.928	0.379	98	43	97	44	58	124 duplicate
10787	26 Citramalic acid	60	Glycerol-3-phosphate	64	-0.168	-0.241	7.148	0.432	99	42	98	45	11	91 original
3234	26 Citramalic acid	108	Octadecanoic acid	64	-0.196	-0.287	17.568	0.367	100	41	100	41	76	129 original
3282	26 Citramalic acid	36	[596; N-Acetylglutamic acid (2TMS)]	64	-0.198	-0.360	14.419	0.374	101	40	103	38	49	126 original
3210	26 Citramalic acid	75	Lysine	64	-0.223	-0.359	24.679	0.383	102	39	102	39	116	122 original
3241	26 Citramalic acid	67	Citric acid	64	-0.239	-0.314	8.465	0.409	103	38	101	40	20	108 original
3240	26 Citramalic acid	66	Glyceric acid-3-phosphate	64	-0.267	-0.428	16.956	0.428	104	37	108	35	70	94 original
3211	26 Citramalic acid	37	Phenylalanine	46	-0.270	-0.390	7.808	0.397	105	36	105	36	14	116 original
3226	26 Citramalic acid	52	[NA]	46	-0.285	-0.456	28.135	0.464	106	35	108	33	129	73 original
3272	26 Citramalic acid	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	48	-0.309	-0.663	28.408	0.529	107	34	128	13	131	28 original
3235	26 Citramalic acid	61	[NA]	64	-0.318	-0.388	14.077	0.442	108	33	104	37	47	86 original
10107	26 Citramalic acid	2	Serine	62	-0.325	-0.433	14.809	0.391	109	32	107	34	55	120 duplicate
3217	26 Citramalic acid	43	[548; Leucine (2TBS)]	60	-0.344	-0.525	12.366	0.420	110	31	111	30	36	98 original
3237	26 Citramalic acid	63	Glutamine	52	-0.356	-0.626	22.965	0.476	111	30	124	17	113	63 original
3263	26 Citramalic acid	89	[775; Dopamine (4TMS)]	35	-0.368	-0.648	22.219	0.412	112	29	127	14	111	102 original
3206	26 Citramalic acid	32	[729; N,N-Dimethyllysine methyl ester]	63	-0.372	-0.639	25.181	0.522	113	28	125	16	119	35 original
3201	26 Citramalic acid	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	-0.388	-0.818	27.530	0.541	114	27	138	3	128	18 original
10245	26 Citramalic acid	3	Ethanolamine	62	-0.389	-0.578	21.757	0.445	115	26	115	26	105	84 duplicate
3205	26 Citramalic acid	31	[822; Parabenic acid (2TMS)]	64	-0.394	-0.647	21.823	0.480	116	25	126	15	106	62 original
3225	26 Citramalic acid	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.402	-0.602	26.638	0.520	117	24	121	20	132	37 original
3269	26 Citramalic acid	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	-0.404	-0.606	29.266	0.443	118	23	122	19	133	85 original
11052	26 Citramalic acid	9	Proline	63	-0.405	-0.474	18.329	0.410	119	22	110	31	85	106 duplicate

12438	26 Citramalic acid	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.415	-0.687	21.824	0.543	120	21	130	11	107	17 duplicate
3242	26 Citramalic acid	68	[570; Hypoxanthine (2TMS)]	20	-0.421	-0.842	20.643	0.430	121	20	140	1	101	92 original
3255	26 Citramalic acid	81	Tyrosine	64	-0.427	-0.594	20.631	0.465	122	19	119	22	100	70 original
3233	26 Citramalic acid	59	Ornithine; Arginine	64	-0.441	-0.541	26.030	0.449	123	18	112	29	123	81 original
3229	26 Citramalic acid	55	[612; 4-Aminobutyric acid (2TBS)]	43	-0.442	-0.588	30.761	0.438	124	17	117	24	137	88 original
3219	26 Citramalic acid	45	Homocysteine	61	-0.444	-0.599	33.016	0.424	125	16	120	21	139	86 original
10920	26 Citramalic acid	8	Isoleucine	55	-0.449	-0.461	13.404	0.388	126	15	109	32	44	121 duplicate
12795	26 Citramalic acid	64	Homoserine	64	-0.450	-0.801	15.764	0.522	127	14	137	4	64	38 duplicate
3251	26 Citramalic acid	77	[626; beta-[[[5-methyl-2-thienyl]methyl]eneamino- benzeneacetic acid methyl ester]	62	-0.452	-0.593	18.359	0.427	128	13	118	23	86	95 original
3207	26 Citramalic acid	33	Methionine	64	-0.457	-0.579	15.777	0.464	129	12	116	25	65	72 original
3204	26 Citramalic acid	30	[815; Ethyl-3(2H)-thiophenone]	64	-0.481	-0.547	17.172	0.410	130	11	113	28	73	107 original
13028	26 Citramalic acid	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.484	-0.761	22.911	0.519	131	10	133	8	112	39 duplicate
3243	26 Citramalic acid	69	Arginine	60	-0.485	-0.780	13.094	0.535	132	9	135	6	40	22 original
3208	26 Citramalic acid	34	Aspartic acid	64	-0.488	-0.555	18.576	0.465	133	8	114	27	89	71 original
3222	26 Citramalic acid	48	Asparagine	64	-0.499	-0.730	17.053	0.497	134	7	132	9	72	52 original
3216	26 Citramalic acid	42	Glutamic acid	60	-0.511	-0.623	19.953	0.440	135	6	123	18	98	87 original
3223	26 Citramalic acid	64	[877; Pyrophosphoric acid (4TMS)]	64	-0.512	-0.680	31.219	0.498	136	5	129	12	138	50 original
11183	26 Citramalic acid	10	Glycine	64	-0.513	-0.781	9.594	0.552	137	4	136	5	23	10 duplicate
3305	26 Citramalic acid	131	[626; 5-Methylthioadenosine (3TMS)]	55	-0.518	-0.701	27.001	0.507	138	3	131	10	126	47 original
3256	26 Citramalic acid	82	Lysine	39	-0.530	-0.837	13.272	0.534	139	2	139	2	42	25 original
10518	26 Citramalic acid	5	Leucine	45	-0.598	-0.778	17.597	0.512	140	1	134	7	77	45 duplicate
10108	27 [815; (E)-4-Methyl-5-hyd	2	Serine	53	0.618	0.670	25.409	0.524	1	140	21	120	89	51 duplicate
12796	27 [815; (E)-4-Methyl-5-hyd	23	Homoserine	53	0.589	0.939	15.859	0.659	2	139	2	139	31	1 duplicate
11053	27 [815; (E)-4-Methyl-5-hyd	9	Proline	52	0.575	0.709	33.981	0.537	3	138	18	123	116	45 duplicate
3319	27 [815; (E)-4-Methyl-5-hyd	31	[622; Parabanic acid (2TMS)]	53	0.559	0.790	12.094	0.550	4	136	10	131	12	37 original
3354	27 [815; (E)-4-Methyl-5-hyd	66	Glycetic acid-3-phosphate	53	0.559	0.739	14.988	0.493	5	137	16	125	24	64 original
3357	27 [815; (E)-4-Methyl-5-hyd	69	Arginine	52	0.516	0.892	27.936	0.618	6	135	4	137	100	8 original
3386	27 [815; (E)-4-Methyl-5-hyd	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	41	0.515	0.769	9.107	0.641	7	134	14	127	3	5 original
3347	27 [815; (E)-4-Methyl-5-hyd	59	Ornithine; Arginine	53	0.509	0.803	48.523	0.551	8	133	8	133	138	35 original
3320	27 [815; (E)-4-Methyl-5-hyd	32	[729; N,N-Dimethyllysine methyl ester]	53	0.502	0.862	10.086	0.857	9	132	6	135	5	2 original
13029	27 [815; (E)-4-Methyl-5-hyd	25	[709; 2,5-Diaminovalerolactam (2TMS)]	37	0.502	0.899	10.768	0.526	10	131	3	138	6	50 duplicate
3321	27 [815; (E)-4-Methyl-5-hyd	33	Methionine	53	0.496	0.790	17.574	0.607	11	130	11	130	42	10 original
3363	27 [815; (E)-4-Methyl-5-hyd	75	Lysine	53	0.485	0.689	47.264	0.471	12	129	20	121	137	76 original
3346	27 [815; (E)-4-Methyl-5-hyd	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	53	0.470	0.627	25.863	0.478	13	128	26	115	93	73 original
10921	27 [815; (E)-4-Methyl-5-hyd	8	Isoleucine	49	0.466	0.583	23.816	0.495	14	127	31	110	81	62 duplicate
3318	27 [815; (E)-4-Methyl-5-hyd	30	[815; Ethyl-3(2H)-thiophenone]	53	0.462	0.800	38.290	0.550	15	126	9	132	124	36 original
3322	27 [815; (E)-4-Methyl-5-hyd	34	Aspartic acid	53	0.457	0.752	41.339	0.608	16	125	15	126	132	11 original
3331	27 [815; (E)-4-Methyl-5-hyd	43	[548; Leucine (2TBS)]	51	0.449	0.561	16.689	0.427	17	124	33	108	34	97 original
11184	27 [815; (E)-4-Methyl-5-hyd	10	Glycine	53	0.421	0.830	27.264	0.591	18	123	7	134	97	14 duplicate
3356	27 [815; (E)-4-Methyl-5-hyd	68	[570; Hypoxanthine (2TMS)]	18	0.412	0.954	6.702	0.568	19	122	1	140	2	22 original
3333	27 [815; (E)-4-Methyl-5-hyd	45	Homocysteine	52	0.398	0.606	13.150	0.540	20	121	27	114	15	42 original
3324	27 [815; (E)-4-Methyl-5-hyd	36	[596; N-Acetylglutamic acid (2TMS)]	53	0.398	0.628	36.996	0.496	21	120	25	116	123	67 original
3369	27 [815; (E)-4-Methyl-5-hyd	81	Tyrosine	53	0.396	0.708	41.716	0.532	22	119	19	122	133	48 original
3365	27 [815; (E)-4-Methyl-5-hyd	77	[626; beta-[[[5-methyl-2-thienyl]methyl]eneamino- benzeneacetic acid methyl ester]	52	0.347	0.735	36.875	0.539	23	118	17	124	122	43 original
3330	27 [815; (E)-4-Methyl-5-hyd	42	Glutamic acid	52	0.345	0.787	36.021	0.581	24	117	13	128	119	17 original
3336	27 [815; (E)-4-Methyl-5-hyd	48	Asparagine	53	0.331	0.645	17.338	0.538	25	116	23	118	38	44 original
10788	27 [815; (E)-4-Methyl-5-hyd	7	Threonine	53	0.321	0.587	39.176	0.522	26	115	30	111	127	52 duplicate

3377	27 [815; (E)-4-Methyl-5-hyd	89	[775; Dopamine (4TMS)]	34	0.305	0.587	11.635	0.443	27	114	28	112	10	93 original
10246	27 [815; (E)-4-Methyl-5-hyd	3	Ethanolamine	52	0.305	0.640	11.631	0.480	28	113	24	117	9	71 duplicate
3337	27 [815; (E)-4-Methyl-5-hyd	49	[877; Pyrophosphoric acid (4TMS)]	53	0.279	0.495	12.575	0.449	29	111	35	106	13	90 original
3325	27 [815; (E)-4-Methyl-5-hyd	37	Phenylalanine	53	0.267	0.588	32.369	0.505	30	112	28	113	112	57 original
3370	27 [815; (E)-4-Methyl-5-hyd	82	Lysine	36	0.257	0.788	19.039	0.590	31	110	12	129	51	15 original
10519	27 [815; (E)-4-Methyl-5-hyd	5	Leucine	43	0.231	0.875	6.328	0.846	32	109	5	136	1	4 duplicate
3419	27 [815; (E)-4-Methyl-5-hyd	131	[626; 5-Methylthioadenosine (3TMS)]	46	0.227	0.538	10.943	0.477	33	108	34	107	7	74 original
10383	27 [815; (E)-4-Methyl-5-hyd	4	Phosphoric acid	45	0.218	0.448	38.361	0.424	34	107	37	104	125	100 duplicate
3351	27 [815; (E)-4-Methyl-5-hyd	63	Glutamine	41	0.207	0.453	16.738	0.457	35	106	36	105	35	82 original
3418	27 [815; (E)-4-Methyl-5-hyd	130	Trehalose	52	0.175	0.303	38.759	0.395	36	105	42	99	126	107 original
3355	27 [815; (E)-4-Methyl-5-hyd	67	Citric acid	53	0.157	0.390	33.468	0.415	37	104	39	102	115	103 original
3352	27 [815; (E)-4-Methyl-5-hyd	64	[789; Tyramine (3TMS)]	52	0.152	-0.001	16.955	0.331	38	103	55	86	38	127 original
11824	27 [815; (E)-4-Methyl-5-hyd	15	Alanine	53	0.145	0.005	28.928	0.567	39	102	54	87	105	23 duplicate
3339	27 [815; (E)-4-Methyl-5-hyd	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	41	0.144	0.665	11.941	0.624	40	101	22	119	11	6 original
3348	27 [815; (E)-4-Methyl-5-hyd	60	Glycerol-3-phosphate	53	0.135	0.323	31.467	0.412	41	100	41	100	111	104 original
3349	27 [815; (E)-4-Methyl-5-hyd	61	[NA]	53	0.134	0.261	17.523	0.380	42	99	46	95	41	113 original
3340	27 [815; (E)-4-Methyl-5-hyd	52	[NA]	37	0.108	0.330	13.315	0.556	43	98	40	101	17	31 original
3367	27 [815; (E)-4-Methyl-5-hyd	79	Glucose	53	0.103	-0.178	43.339	0.450	44	97	61	80	136	89 original
3360	27 [815; (E)-4-Methyl-5-hyd	72	[918; D-Xylopyranose (4TMS)]	53	0.075	0.125	16.377	0.314	45	96	48	93	33	130 original
3383	27 [815; (E)-4-Methyl-5-hyd	95	[770; 3,4,6-Trisubstitutedphenylethandiamine (5TMS)]	44	0.074	0.417	13.426	0.457	46	95	38	103	19	83 original
3396	27 [815; (E)-4-Methyl-5-hyd	108	Octadecenoic acid	53	0.057	0.297	15.647	0.376	47	94	43	98	28	114 original
3371	27 [815; (E)-4-Methyl-5-hyd	83	Sorbitol	49	0.029	0.272	28.603	0.480	48	93	45	96	103	70 original
3406	27 [815; (E)-4-Methyl-5-hyd	118	[928; Glucopyranose-6-phosphate (6TMS)]	47	0.018	-0.138	18.114	0.310	49	92	60	81	44	132 original
3343	27 [815; (E)-4-Methyl-5-hyd	55	[612; 4-Aminobutyric acid (2TMS)]	38	0.010	0.282	15.818	0.530	50	91	44	97	29	49 original
3411	27 [815; (E)-4-Methyl-5-hyd	123	[945; Galactofuranose-6-phosphate (7TMS)]	53	0.001	-0.206	22.841	0.419	51	90	64	77	76	102 original
3427	27 [815; (E)-4-Methyl-5-hyd	136	[700; Ergosta-5,7-dien-3-ol]	30	-0.016	0.025	11.201	0.223	52	89	51	90	8	137 original
3424	27 [815; (E)-4-Methyl-5-hyd	71	[748; D-Sedoheptulose-7-phosphate (7TMS)]	13	-0.026	0.192	13.381	0.096	53	88	47	94	18	140 original
3359	27 [815; (E)-4-Methyl-5-hyd	131	[731; Erythrose (3TMS)]	53	-0.039	0.021	23.673	0.466	54	87	52	89	80	77 original
3335	27 [815; (E)-4-Methyl-5-hyd	47	[NA]	53	-0.042	-0.133	20.521	0.388	55	86	58	83	60	112 original
3341	27 [815; (E)-4-Methyl-5-hyd	53	Glycerol-2-phosphate	53	-0.049	0.096	14.182	0.311	56	85	50	91	23	131 original
3421	27 [815; (E)-4-Methyl-5-hyd	133	[855; Squalene]	53	-0.061	-0.041	19.107	0.368	57	84	56	85	52	115 original
3368	27 [815; (E)-4-Methyl-5-hyd	80	[772; D-Glucose (5TMS)]	51	-0.098	-0.373	39.433	0.389	58	83	71	70	128	109 original
3384	27 [815; (E)-4-Methyl-5-hyd	86	myo-Inositol	42	-0.099	-0.204	14.014	0.253	59	82	62	79	22	134 original
3401	27 [815; (E)-4-Methyl-5-hyd	113	Galactose-6-phosphate	51	-0.117	-0.447	19.181	0.361	60	81	78	63	53	118 original
3392	27 [815; (E)-4-Methyl-5-hyd	104	[795; Erythritol (4TMS)]	52	-0.121	-0.381	19.320	0.454	61	80	72	69	54	87 original
3398	27 [815; (E)-4-Methyl-5-hyd	111	[583; Erythritol (4TMS)]	34	-0.127	-0.231	13.119	0.204	62	79	66	75	14	139 original
3412	27 [815; (E)-4-Methyl-5-hyd	124	[734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]	48	-0.145	0.123	15.454	0.351	63	78	49	92	28	123 original
3407	27 [815; (E)-4-Methyl-5-hyd	119	[931; myo-Inositol-2-phosphate (7TMS)]	53	-0.149	-0.138	19.969	0.356	64	77	59	82	57	122 original
3389	27 [815; (E)-4-Methyl-5-hyd	101	[832; Dopamine (4TMS)]	53	-0.151	-0.584	22.664	0.487	65	76	89	52	75	66 original
3329	27 [815; (E)-4-Methyl-5-hyd	41	[639; Proline (2TMS)]	53	-0.163	-0.440	25.754	0.402	66	75	76	65	91	106 original
10654	27 [815; (E)-4-Methyl-5-hyd	6	Glycerol	53	-0.165	-0.400	49.290	0.360	67	74	74	67	140	120 duplicate
3375	27 [815; (E)-4-Methyl-5-hyd	87	[945; beta-D-Glucopyranose (5TMS)]	51	-0.191	-0.447	42.498	0.356	68	73	77	64	134	121 original
3379	27 [815; (E)-4-Methyl-5-hyd	91	[766; beta-D-Methylglucopyranoside (4TMS)]	53	-0.192	-0.567	26.375	0.448	69	72	87	54	98	91 original
3402	27 [815; (E)-4-Methyl-5-hyd	114	Fructose-6-phosphate	42	-0.192	-0.514	18.197	0.328	70	71	84	57	45	128 original
3361	27 [815; (E)-4-Methyl-5-hyd	73	[708; Glucose methoxamine (5TMS)]	49	-0.197	-0.594	20.113	0.497	71	70	93	48	59	61 original
3381	27 [815; (E)-4-Methyl-5-hyd	93	[607; Putrescine (4TMS)]	49	-0.199	-0.265	16.159	0.428	72	69	67	74	32	98 original
3425	27 [815; (E)-4-Methyl-5-hyd	137	Ergosterol	53	-0.210	0.018	24.512	0.387	73	68	53	88	84	110 original
12439	27 [815; (E)-4-Methyl-5-hyd	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	30	-0.214	0.567	9.852	0.649	74	67	32	109	4	3 duplicate
3413	27 [815; (E)-4-Methyl-5-hyd	125	[892; Sucrose (8TMS); alpha-D-Glc(1,2)-beta-D-Fru]	53	-0.215	-0.487	41.023	0.420	75	66	81	60	130	101 original

12186	27 [815; (E)-4-Methyl-5-hyd	18	[590; 1-Acetyl-2-thiopyranoside]	53	-0.216	-0.579	20,804	0.460	76	65	88	53	62	81 duplicate
12318	27 [815; (E)-4-Methyl-5-hyd	19	[Alanine (BP) (3TMS)]	53	-0.218	-0.505	24,748	0.432	77	64	83	58	87	95 duplicate
3426	27 [815; (E)-4-Methyl-5-hyd	138	[674; Ergosterol (1TMS)]	36	-0.222	-0.206	13,304	0.306	78	63	63	78	16	133 original
3395	27 [815; (E)-4-Methyl-5-hyd	107	9-(Z)-Octadecenoic acid	53	-0.235	-0.073	25,817	0.332	79	62	57	84	92	126 original
3323	27 [815; (E)-4-Methyl-5-hyd	35	Pyroglutamic acid	53	-0.237	-0.585	49,011	0.457	80	61	90	51	139	88 original
3358	27 [815; (E)-4-Methyl-5-hyd	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	48	-0.245	-0.329	27,952	0.381	81	60	69	72	101	119 original
3391	27 [815; (E)-4-Methyl-5-hyd	103	[648; Ethylamine (2TMS)]	52	-0.249	-0.680	25,915	0.519	82	59	102	39	94	54 original
3408	27 [815; (E)-4-Methyl-5-hyd	120	[945; Uridine (3TMS)]	43	-0.267	-0.226	23,611	0.538	83	58	65	76	79	47 original
3403	27 [815; (E)-4-Methyl-5-hyd	115	Glucose-6-phosphate	51	-0.274	-0.592	35,101	0.444	84	57	92	49	118	92 original
3368	27 [815; (E)-4-Methyl-5-hyd	78	Mannitol	52	-0.278	-0.613	20,966	0.464	85	56	86	45	64	78 original
3372	27 [815; (E)-4-Methyl-5-hyd	84	Mannitol	52	-0.279	-0.584	39,703	0.457	86	55	86	55	129	85 original
9969	27 [815; (E)-4-Methyl-5-hyd	1	[938; Sulfuric acid (2TMS)]	25	-0.293	-0.488	17,897	0.216	87	54	82	59	43	138 duplicate
3376	27 [815; (E)-4-Methyl-5-hyd	88	Gluconic acid	53	-0.295	-0.728	24,989	0.564	88	53	110	31	88	27 original
3328	27 [815; (E)-4-Methyl-5-hyd	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	53	-0.298	-0.865	21,558	0.582	89	52	137	4	68	16 original
3364	27 [815; (E)-4-Methyl-5-hyd	76	Fructose	53	-0.298	-0.621	36,043	0.491	90	51	98	43	120	65 original
3374	27 [815; (E)-4-Methyl-5-hyd	86	[793; D-Galactono-1,4-lactone (4TMS)]	53	-0.299	-0.714	34,558	0.546	91	50	108	33	117	39 original
3429	27 [815; (E)-4-Methyl-5-hyd	141	[Lanosta-8,24-dien-3-beta-ol	51	-0.307	-0.343	15,835	0.393	92	49	70	71	30	108 original
12559	27 [815; (E)-4-Methyl-5-hyd	21	[678; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	28	-0.312	-0.818	19,412	0.253	94	47	97	44	58	135 original
12073	27 [815; (E)-4-Methyl-5-hyd	17	[700; 2-methyl-1,2-propanediol (2TMS)]	53	-0.315	-0.748	29,442	0.499	95	46	115	26	108	58 duplicate
3378	27 [815; (E)-4-Methyl-5-hyd	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	53	-0.319	-0.283	20,058	0.336	96	45	68	73	58	125 original
12913	27 [815; (E)-4-Methyl-5-hyd	24	[725; 2-Ketodecanoic acid (2TMS)]	53	-0.329	-0.836	41,202	0.564	97	44	128	12	131	26 duplicate
3385	27 [815; (E)-4-Methyl-5-hyd	97	[756; beta-D-Methylglucopyranoside (4TMS)]	44	-0.332	-0.588	31,162	0.366	98	43	91	50	110	118 original
3394	27 [815; (E)-4-Methyl-5-hyd	106	[733; Threitol (4TMS)]	51	-0.333	-0.720	24,382	0.548	99	42	109	32	83	38 original
3422	27 [815; (E)-4-Methyl-5-hyd	134	Isomaltose	53	-0.337	-0.800	36,081	0.574	100	41	125	16	121	19 original
3344	27 [815; (E)-4-Methyl-5-hyd	56	[828; Orotic acid (3TMS)]	53	-0.340	-0.780	23,163	0.566	101	40	121	20	77	24 original
11949	27 [815; (E)-4-Methyl-5-hyd	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	53	-0.343	-0.853	29,543	0.571	102	39	134	7	108	21 duplicate
3328	27 [815; (E)-4-Methyl-5-hyd	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	53	-0.344	-0.769	42,852	0.597	103	38	119	22	135	13 original
3350	27 [815; (E)-4-Methyl-5-hyd	62	[812; D-Xylofuranose (4TMS)]	53	-0.347	-0.728	26,036	0.555	104	37	111	30	95	32 original
3397	27 [815; (E)-4-Methyl-5-hyd	109	Octadecanoic acid	53	-0.348	-0.458	33,265	0.408	105	36	79	62	114	105 original
3373	27 [815; (E)-4-Methyl-5-hyd	85	[528; Methylchloric acid (4TMS)]	44	-0.353	-0.737	13,432	0.551	106	35	112	29	20	34 original
3334	27 [815; (E)-4-Methyl-5-hyd	46	Arabinose	53	-0.354	-0.763	30,234	0.565	107	33	117	24	109	25 original
3317	27 [815; (E)-4-Methyl-5-hyd	28	Erythritol	53	-0.354	-0.851	18,681	0.605	108	34	133	8	49	12 original
3409	27 [815; (E)-4-Methyl-5-hyd	121	[657; Erythritol (4TMS)]	44	-0.355	-0.683	18,207	0.479	109	32	103	38	46	72 original
3428	27 [815; (E)-4-Methyl-5-hyd	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	40	-0.356	-0.397	13,626	0.364	110	31	73	68	21	117 original
3353	27 [815; (E)-4-Methyl-5-hyd	65	[646; 3-Deoxyglucitol (5TMS)]	52	-0.360	-0.804	25,688	0.557	111	30	126	15	90	30 original
3414	27 [815; (E)-4-Methyl-5-hyd	126	[559; Erythritol (4TMS)]	34	-0.365	-0.596	19,326	0.457	112	29	94	47	55	84 original
3382	27 [815; (E)-4-Methyl-5-hyd	94	Hexadecanoic acid	53	-0.366	-0.429	32,552	0.387	113	28	75	66	113	111 original
3405	27 [815; (E)-4-Methyl-5-hyd	117	[724; Glycerol (3TMS)]	45	-0.372	-0.743	21,191	0.494	114	27	114	27	65	63 original
3327	27 [815; (E)-4-Methyl-5-hyd	39	[829; 1-Phenylethanol (1TMS)]	52	-0.373	-0.860	29,499	0.571	115	26	135	6	107	20 original
3360	27 [815; (E)-4-Methyl-5-hyd	92	[680; Glycerol-2-phosphate (4TMS)]	43	-0.378	-0.473	20,836	0.326	116	25	80	61	63	128 original
		129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]											
3417	27 [815; (E)-4-Methyl-5-hyd	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	48	-0.379	-0.776	24,546	0.460	117	24	120	21	85	80 original
3416	27 [815; (E)-4-Methyl-5-hyd	140	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	34	-0.380	-0.668	22,644	0.342	118	23	101	40	74	124 original
3332	27 [815; (E)-4-Methyl-5-hyd	44	[715; Erythritol (4TMS)]	43	-0.382	-0.654	23,300	0.454	119	22	99	42	78	88 original
3398	27 [815; (E)-4-Methyl-5-hyd	110	Succinic acid	53	-0.384	-0.705	22,505	0.522	120	21	107	34	73	53 original
11314	27 [815; (E)-4-Methyl-5-hyd	26	Citramalic acid	53	-0.388	-0.798	21,298	0.540	121	19	124	17	68	41 duplicate
13144	27 [815; (E)-4-Methyl-5-hyd	122	[644; Erythritol (4TMS)]	53	-0.388	-0.818	27,530	0.541	122	20	127	14	99	40 duplicate
3410	27 [815; (E)-4-Methyl-5-hyd	122	[644; Erythritol (4TMS)]	41	-0.388	-0.760	21,307	0.499	123	18	122	19	67	59 original
3316	27 [815; (E)-4-Methyl-5-hyd	28	Malic acid	53	-0.389	-0.869	22,463	0.617	124	17	138	3	72	9 original
3390	27 [815; (E)-4-Methyl-5-hyd	102	[904; Galactose methoxyamine (5TMS)]	53	-0.393	-0.612	17,505	0.484	125	16	95	46	40	68 original

3338	27 [815; (E)-4-Methyl-5-hyd	50	-0.401	-0.844	18.635	0.537	126	15	131	10	48	46 original
11571	27 [815; (E)-4-Methyl-5-hyd	13	-0.403	-0.863	28.822	0.580	127	14	136	5	104	18 duplicate
3420	27 [815; (E)-4-Methyl-5-hyd	132	-0.406	-0.844	21.662	0.441	128	13	132	9	69	94 original
11898	27 [815; (E)-4-Methyl-5-hyd	14	-0.409	-0.874	17.354	0.622	129	12	139	2	39	7 duplicate
3382	27 [815; (E)-4-Methyl-5-hyd	74	-0.422	-0.657	22.155	0.505	130	10	100	41	71	56 original
3388	27 [815; (E)-4-Methyl-5-hyd	100	-0.422	-0.686	21.742	0.472	131	11	104	37	70	75 original
12678	27 [815; (E)-4-Methyl-5-hyd	22	-0.432	-0.881	18.763	0.553	132	9	140	1	50	33 duplicate
3423	27 [815; (E)-4-Methyl-5-hyd	902; Melibiose (8TMS);	-0.440	-0.695	24.062	0.484	133	8	105	36	82	69 original
3342	27 [815; (E)-4-Methyl-5-hyd	54 [NA]	-0.444	-0.759	20.705	0.461	134	7	116	25	61	79 original
3400	27 [815; (E)-4-Methyl-5-hyd	112	-0.451	-0.704	15.138	0.498	135	6	108	35	25	60 original
3393	27 [815; (E)-4-Methyl-5-hyd	105	-0.456	-0.737	24.655	0.432	136	5	113	28	86	96 original
3387	27 [815; (E)-4-Methyl-5-hyd	99	-0.457	-0.839	18.506	0.426	137	4	130	11	47	99 original
3345	27 [815; (E)-4-Methyl-5-hyd	757; 2-Desoxy-pentos-3-yose dimethoxyamine (2TMS)]	-0.461	-0.768	27.293	0.514	138	3	118	23	98	55 original
11443	27 [815; (E)-4-Methyl-5-hyd	12	-0.475	-0.832	17.099	0.563	139	2	128	13	37	28 duplicate
3404	27 [815; (E)-4-Methyl-5-hyd	116	-0.514	-0.845	15.590	0.243	140	1	85	56	27	136 original
11699	28 Malic acid	14	0.825	0.978	11.647	0.681	1	140	1	140	55	2 duplicate
11315	28 Malic acid	11	0.736	0.919	2.576	0.604	2	139	11	130	2	30 duplicate
3516	28 Malic acid	115	0.731	0.834	16.978	0.588	3	138	34	107	80	37 original
12679	28 Malic acid	22	0.710	0.940	14.610	0.610	4	137	3	138	73	28 duplicate
3441	28 Malic acid	40	0.706	0.910	27.109	0.645	5	136	14	127	131	14 original
3477	28 Malic acid	76	0.690	0.845	18.088	0.603	6	135	31	110	97	31 original
3439	28 Malic acid	38	0.684	0.960	3.094	0.663	7	134	2	139	3	8 original
3463	28 Malic acid	62	0.674	0.885	5.819	0.625	8	133	20	121	12	18 original
3501	28 Malic acid	100	0.672	0.857	2.023	0.560	9	132	27	114	1	54 original
3438	28 Malic acid	35	0.671	0.830	33.900	0.584	10	131	35	106	138	17 original
3430	28 Malic acid	29	0.668	0.928	6.368	0.630	11	130	7	134	15	43 duplicate
12560	28 Malic acid	21	0.666	0.851	8.469	0.579	12	129	30	111	29	19 duplicate
11444	28 Malic acid	63	0.658	0.912	13.927	0.625	13	128	13	128	68	12 duplicate
12914	28 Malic acid	24	0.655	0.831	24.404	0.654	14	127	6	135	122	11 original
3507	28 Malic acid	106	0.653	0.876	7.703	0.654	15	126	22	119	23	7 duplicate
11950	28 Malic acid	16	0.647	0.927	9.735	0.663	16	125	8	133	36	9 original
3487	28 Malic acid	86	0.639	0.880	17.197	0.661	17	124	21	120	92	25 duplicate
13145	28 Malic acid	26	0.637	0.863	8.452	0.612	18	123	25	116	28	56 original
3503	28 Malic acid	102	0.634	0.796	8.580	0.556	19	122	41	100	30	3 original
3479	28 Malic acid	39	0.620	0.937	10.475	0.680	20	121	4	137	43	47 original
3457	28 Malic acid	78	0.617	0.827	12.277	0.577	21	120	37	104	59	5 original
3522	28 Malic acid	56	0.614	0.902	12.232	0.665	22	119	15	126	58	50 original
3518	28 Malic acid	121	0.605	0.814	16.897	0.566	23	118	39	102	89	53 original
3523	28 Malic acid	117	0.604	0.858	9.491	0.563	24	117	26	115	33	48 original
3513	28 Malic acid	122	0.599	0.888	18.064	0.574	25	116	18	123	96	61 original
11572	28 Malic acid	112	0.595	0.829	20.137	0.545	26	115	36	105	105	10 original
3535	28 Malic acid	13	0.595	0.921	8.731	0.663	27	114	10	131	31	65 original
3455	28 Malic acid	134	0.593	0.918	18.003	0.658	28	113	12	129	95	1 original
3466	28 Malic acid	65	0.589	0.857	14.385	0.536	29	112	28	113	70	1 original
3533	28 Malic acid	132	0.584	0.926	14.020	0.694	30	111	9	132	69	44 original
3447	28 Malic acid	42	0.584	0.937	17.725	0.578	31	110	5	136	93	13 original
3511	28 Malic acid	64	0.582	0.895	12.770	0.649	32	109	17	124	63	20 original
3515	28 Malic acid	110	0.575	0.844	13.314	0.623	33	108	32	109	66	68 original
		114	0.570	0.770	11.203	0.529	34	107	42	99	49	

3471	28 Malic acid	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	0.569	0.581	11,645	0.457	35	106	58	83	54	97 original
3526	28 Malic acid	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	0.566	0.720	24,552	0.537	36	105	49	92	124	64 original
3458	28 Malic acid	73	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55	0.561	0.871	11,201	0.593	37	104	23	118	48	35 original
3474	28 Malic acid	73	[708; Glucose methoxyamine (5TMS)]	57	0.559	0.769	11,232	0.507	38	103	43	98	50	78 original
3527	28 Malic acid	126	[559; Erythritol (4TMS)]	45	0.556	0.764	10,240	0.546	39	102	45	96	41	59 original
12074	28 Malic acid	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	0.553	0.856	9,920	0.566	40	101	29	112	38	51 duplicate
3530	28 Malic acid	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	0.552	0.896	11,043	0.603	41	100	16	125	47	32 original
3451	28 Malic acid	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	0.550	0.888	22,017	0.612	42	99	19	122	108	28 original
3536	28 Malic acid	135	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	0.544	0.754	4,408	0.526	43	98	46	95	6	69 original
3445	28 Malic acid	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	0.543	0.801	8,241	0.539	44	97	40	101	27	62 original
3486	28 Malic acid	85	[529; Methylcitric acid (4TMS)]	48	0.543	0.818	4,638	0.565	45	96	38	103	7	52 original
3475	28 Malic acid	74	[912; Tetradecanoic acid (1TMS)]	64	0.540	0.767	10,579	0.496	46	95	44	97	44	80 original
3489	28 Malic acid	88	Gluconic acid	64	0.539	0.863	6,868	0.622	47	94	24	117	17	21 original
3521	28 Malic acid	120	[945; Uridine (3TMS)]	54	0.533	0.342	5,750	0.599	48	93	73	68	11	33 original
12197	28 Malic acid	18	[590; 1-Acetyl-2-thiondantoin]	64	0.527	0.685	3,620	0.486	49	92	51	90	4	86 duplicate
3514	28 Malic acid	116	[882; Pseudouridine (5TMS)]	30	0.476	0.538	9,771	0.451	50	91	50	91	45	91 original
3517	28 Malic acid	92	[680; Glycerol-2-phosphate (4TMS)]	54	0.458	0.639	9,576	0.488	52	89	62	79	37	102 original
3493	28 Malic acid	19	Alanine (BP) (3TMS)	64	0.441	0.649	5,447	0.494	53	88	54	87	10	85 original
12319	28 Malic acid	103	[648; Ethylamine (2TMS)]	63	0.438	0.720	11,473	0.546	54	87	48	93	52	81 duplicate
3529	28 Malic acid	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.406	0.748	6,074	0.522	55	86	47	94	13	60 original
3528	28 Malic acid	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.379	0.664	7,053	0.556	56	85	53	88	18	72 original
3512	28 Malic acid	111	[583; Erythritol (4TMS)]	42	0.370	0.497	23,358	0.394	57	84	65	76	118	55 original
10655	28 Malic acid	6	Glycerol	64	0.366	0.582	34,518	0.452	58	82	57	84	140	101 duplicate
3524	28 Malic acid	123	[945; Galactofuranose-6-phosphate (7TMS)]	64	0.366	0.478	4,202	0.476	59	83	68	73	5	90 original
3484	28 Malic acid	83	Sorbitol	58	0.358	-0.156	15,383	0.391	60	81	92	49	78	132 original
3505	28 Malic acid	104	[795; Erythritol (4TMS)]	63	0.346	0.488	7,648	0.467	61	80	67	74	22	94 original
3442	28 Malic acid	41	[638; Proline (2TMS)]	64	0.343	0.517	6,456	0.483	62	79	63	78	16	87 original
3497	28 Malic acid	96	myo-Inositol	49	0.335	0.296	22,341	0.345	63	78	74	67	112	139 original
3502	28 Malic acid	101	[832; Dopamine (4TMS)]	64	0.317	0.574	9,258	0.458	64	77	59	82	32	98 original
3482	28 Malic acid	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	0.300	0.515	15,566	0.451	65	76	64	77	78	104 original
3488	28 Malic acid	87	[945; beta-D-Glucopyranose (5TMS)]	62	0.291	0.594	28,219	0.479	66	75	56	85	135	88 original
3506	28 Malic acid	105	[705; 2-Ketogluconic acid (5TMS)]	48	0.287	0.687	9,637	0.539	67	74	52	89	35	63 original
3498	28 Malic acid	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	0.281	0.574	16,003	0.421	68	73	60	81	83	121 original
3541	28 Malic acid	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	49	0.272	0.365	18,578	0.451	69	72	72	69	98	103 original
3534	28 Malic acid	133	[855; Squalene]	64	0.269	0.172	7,767	0.381	70	71	81	60	24	135 original
3510	28 Malic acid	109	Octadecanoic acid	64	0.255	0.559	15,956	0.468	71	70	61	80	82	93 original
3465	28 Malic acid	64	[789; Tyramine (3TMS)]	63	0.248	0.245	7,626	0.416	72	69	78	63	20	122 original
3539	28 Malic acid	138	[674; Ergosterol (1TMS)]	46	0.219	0.269	19,308	0.422	73	68	76	65	102	120 original
11825	28 Malic acid	15	Alanine	64	0.210	0.226	11,845	0.590	74	67	79	62	57	36 duplicate
3495	28 Malic acid	94	Hexadecanoic acid	64	0.208	0.489	14,520	0.445	75	66	66	75	72	107 original
3500	28 Malic acid	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	0.195	0.841	13,108	0.577	76	65	63	108	64	45 original
3480	28 Malic acid	79	Glucose	64	0.182	0.442	27,741	0.511	77	64	70	71	134	75 original
3481	28 Malic acid	80	[772; D-Glucose (5TMS)]	62	0.176	0.465	23,851	0.422	78	63	69	72	120	119 original
3542	28 Malic acid	141	Lanosta-8,24-dien-3-beta-ol	61	0.151	0.263	17,033	0.470	79	62	77	64	91	92 original
3485	28 Malic acid	84	Mannitol	62	0.119	0.387	24,923	0.444	80	61	71	70	126	110 original
3537	28 Malic acid	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.118	0.027	5,111	0.445	81	60	86	55	8	108 original
3538	28 Malic acid	137	Ergosterol	64	0.097	0.043	10,185	0.442	82	59	85	56	40	111 original

3540	28 Malic acid	139	[700; Ergosta-5,7-dien-3-ol]	38	0.084	-0.006	21,023	0.393	83	58	89	52	107	131 original
3472	28 Malic acid	71	[731; Erythrose (3TMS)]	64	0.075	-0.005	5,346	0.427	84	57	88	53	9	116 original
3491	28 Malic acid	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	64	0.027	0.049	6,280	0.373	85	56	83	58	14	136 original
3519	28 Malic acid	118	[928; Glucopyranose-6-phosphate (6TMS)]	58	0.019	0.089	11,778	0.406	86	55	82	59	56	124 original
3494	28 Malic acid	93	[607; Putrescine (4TMS)]	60	0.016	0.198	19,983	0.368	87	54	80	61	103	137 original
		124	[734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]	59	-0.023	-0.176	27,250	0.404	88	53	93	48	132	127 original
3525	28 Malic acid	119	[931; myo-Inositol-2-phosphate (7TMS)]	64	-0.029	0.046	7,634	0.428	89	52	84	57	21	115 original
3520	28 Malic acid	107	9-(Z)-Octadecenoic acid	64	-0.043	-0.122	7,976	0.384	90	51	90	51	26	133 original
3508	28 Malic acid	47	[NA]	64	-0.047	0.001	11,639	0.456	91	50	87	54	53	98 original
3448	28 Malic acid	1	[938; Sulfuric acid (2TMS)]	36	-0.048	0.277	10,364	0.498	92	49	75	66	42	79 duplicate
9970	28 Malic acid	53	Glycerol-2-phosphate	64	-0.070	-0.130	14,483	0.342	93	48	91	50	71	140 original
3454	28 Malic acid	7	Threonine	64	-0.103	-0.383	23,216	0.449	94	47	99	42	117	106 duplicate
10789	28 Malic acid	130	Trehalose	63	-0.153	-0.312	22,870	0.383	95	46	95	46	116	134 original
3531	28 Malic acid	4	Phosphoric acid	51	-0.170	-0.343	27,450	0.401	96	45	97	44	133	128 duplicate
10384	28 Malic acid	58	[636; 4R-Acetamidol-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	-0.198	-0.384	11,310	0.412	97	44	100	41	51	123 original
3459	28 Malic acid	75	Lysine	64	-0.199	-0.460	32,940	0.425	98	43	103	38	137	117 original
3476	28 Malic acid	36	[596; N-Acetylglutamic acid (2TMS)]	64	-0.206	-0.472	22,275	0.424	99	42	104	37	110	118 original
3468	28 Malic acid	67	Citric acid	64	-0.219	-0.401	16,702	0.404	100	41	101	40	86	126 original
3473	28 Malic acid	72	[919; D-Xylopyranose (4TMS)]	63	-0.222	-0.269	12,373	0.364	101	40	94	47	60	138 original
3461	28 Malic acid	60	Glycerol-3-phosphate	64	-0.231	-0.377	14,756	0.455	102	39	98	43	75	99 original
3438	28 Malic acid	37	Phenylalanine	64	-0.242	-0.510	15,876	0.442	103	38	106	35	81	112 original
3467	28 Malic acid	66	Glyceric acid-3-phosphate	64	-0.249	-0.552	10,088	0.490	104	37	109	32	39	84 original
3509	28 Malic acid	108	Octadecenoic acid	64	-0.262	-0.407	10,870	0.404	105	36	102	39	48	125 original
3462	28 Malic acid	61	[NA]	64	-0.273	-0.341	7,613	0.450	106	35	96	45	19	105 original
10109	28 Malic acid	2	Serine	62	-0.290	-0.535	16,769	0.444	107	34	107	34	87	109 duplicate
3453	28 Malic acid	52	[NA]	46	-0.326	-0.577	22,735	0.585	108	33	110	31	115	39 original
10922	28 Malic acid	8	Isoleucine	55	-0.329	-0.479	16,027	0.398	109	32	105	36	84	129 duplicate
11054	28 Malic acid	9	Proline	60	-0.332	-0.577	23,705	0.436	110	31	111	30	119	114 duplicate
3444	28 Malic acid	43	[548; Leucine (2TBS)]	60	-0.337	-0.551	7,882	0.477	111	30	108	33	25	89 original
3499	28 Malic acid	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	48	-0.340	-0.822	22,205	0.599	112	29	132	9	109	34 original
3432	28 Malic acid	31	[822; Parabanic acid (2TMS)]	64	-0.362	-0.688	14,898	0.533	113	28	121	20	76	67 original
3464	28 Malic acid	63	Glutamine	52	-0.386	-0.671	19,162	0.620	114	27	119	22	101	22 original
13259	28 Malic acid	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	-0.389	-0.869	22,463	0.617	115	26	134	7	114	23 duplicate
12797	28 Malic acid	23	Homoserine	64	-0.393	-0.883	12,699	0.605	116	25	136	5	62	29 duplicate
3435	28 Malic acid	34	Aspartic acid	64	-0.415	-0.611	26,533	0.512	117	24	112	29	130	74 original
10247	28 Malic acid	3	Ethanolamine	62	-0.419	-0.700	15,334	0.534	118	23	123	18	77	66 duplicate
3434	28 Malic acid	33	Methionine	64	-0.424	-0.670	12,392	0.522	119	22	118	23	61	71 original
3452	28 Malic acid	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.429	-0.733	22,297	0.551	120	21	125	16	111	58 original
3431	28 Malic acid	30	[815; Ethyl-3(2H)-thiophenone]	64	-0.439	-0.652	24,432	0.455	121	20	116	25	123	100 original
3469	28 Malic acid	68	[570; Hypoxanthine (2TMS)]	20	-0.442	-0.941	16,300	0.588	122	19	140	1	85	38 original
3433	28 Malic acid	32	[729; N,N-Dimethyllysine methyl ester]	63	-0.446	-0.778	20,266	0.616	123	18	129	12	106	24 original
3446	28 Malic acid	45	Homocysteine	61	-0.457	-0.644	25,521	0.459	124	17	114	27	128	85 original
	28 Malic acid													
2440	28 Malic acid	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.458	-0.769	16,854	0.675	125	16	128	13	88	4 duplicate
3460	28 Malic acid	59	Ornithine; Arginine	64	-0.461	-0.651	34,323	0.494	126	15	115	26	139	82 original
3456	28 Malic acid	55	[612; 4-Aminobutyric acid (2TBS)]	43	-0.464	-0.655	24,299	0.526	127	14	117	24	121	70 original
3496	28 Malic acid	95	[770; 3,4,6-Tris(hydroxyphenyl)ethanolamine (5TMS)]	50	-0.464	-0.643	22,360	0.438	128	13	113	28	113	113 original
		77	[826; beta-[[[5-methyl-2-thienyl)methyl]amino-benzeneacetic acid methyl ester]	62	-0.465	-0.695	25,082	0.508	129	12	122	19	127	77 original



3482	28 Malic acid	81 Tyrosine	64 -0.488	-0.737	28.390	0.566	130	11	126	15	136	49 original
3449	28 Malic acid	42 Asparagine	64 -0.501	-0.785	13.873	0.577	131	10	130	11	67	46 original
3443	28 Malic acid	40 Glutamic acid	60 -0.507	-0.724	25.930	0.510	132	9	124	17	129	78 original
13030	28 Malic acid	25 [709; 2,5-Diaminovalerolactam (2TMS)]	48 -0.512	-0.900	19.106	0.551	133	8	137	4	100	57 duplicate
3470	28 Malic acid	69 Arginine	60 -0.519	-0.870	17.949	0.610	134	7	135	6	94	27 original
3450	28 Malic acid	49 [877; Pyrophosphoric acid (4TMS)]	64 -0.538	-0.676	24.669	0.493	135	6	120	21	125	83 original
10520	28 Malic acid	5 Leucine	45 -0.545	-0.851	13.186	0.583	136	5	133	8	65	41 duplicate
3480	28 Malic acid	89 [775; Dopamine (4TMS)]	35 -0.553	-0.804	19.058	0.581	137	4	131	10	99	42 original
3532	28 Malic acid	131 [626; 5-Methylthioadenosine (3TMS)]	55 -0.556	-0.740	20.075	0.519	138	3	127	14	104	73 original
11885	28 Malic acid	10 Glycine	64 -0.578	-0.903	14.662	0.638	139	2	138	3	74	16 duplicate
3483	28 Malic acid	82 Lysine	39 -0.622	-0.915	15.865	0.645	140	1	139	2	80	15 original
11951	29 Erythritol	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	64 -0.846	0.982	15.701	0.693	1	140	1	140	83	1 duplicate
12915	29 Erythritol	24 [725; 2-Ketocacetic acid (2TMS)]	64 -0.842	0.971	30.557	0.653	2	139	3	138	130	10 duplicate
3551	29 Erythritol	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	64 -0.794	0.974	4.208	0.671	3	138	2	139	6	2 original
3552	29 Erythritol	39 [829; 1-Phenylethanol (1TMS)]	63 -0.789	0.982	14.074	0.660	4	137	4	137	74	5 original
3559	29 Erythritol	46 Arabinose	64 -0.780	0.924	15.591	0.662	5	136	17	124	82	3 original
11316	29 Erythritol	11 Succinic acid	64 -0.778	0.940	4.369	0.650	6	135	9	132	7	13 duplicate
12075	29 Erythritol	17 [700; 2-methyl-1,2-propanediol (2TMS)]	64 -0.776	0.931	15.513	0.615	7	134	12	129	80	29 duplicate
3599	29 Erythritol	86 [793; D-Galactono-1,4-lactone (4TMS)]	61 -0.774	0.891	20.335	0.635	8	133	21	120	108	20 original
3570	29 Erythritol	[757; 2-Desoxy-pentos-3-ylose dimethoxyamine (2TMS)]	55 -0.774	0.896	12.219	0.634	9	132	20	121	62	21 original
3569	29 Erythritol	56 [829; Orotic acid (3TMS)]	64 -0.768	0.932	8.891	0.641	10	131	11	130	39	17 original
3578	29 Erythritol	65 [846; 3-Deoxyglucitol (5TMS)]	63 -0.768	0.942	11.698	0.652	11	130	7	134	55	11 original
129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]											
134	Isomaltose		59 -0.759	0.930	9.756	0.585	12	129	13	128	44	48 original
13	Uracil		64 -0.755	0.938	23.288	0.643	13	128	10	131	118	16 original
50	[746; Ribonic acid-1,4-lactone (3TMS)]		64 -0.753	0.959	14.004	0.657	14	127	5	136	73	6 duplicate
54	[NA]		61 -0.734	0.941	16.038	0.649	15	126	8	133	86	14 original
12	Glyceric acid		55 -0.717	0.903	9.690	0.580	16	125	19	122	43	50 original
88	Gluconic acid		63 -0.701	0.929	7.821	0.606	17	124	15	128	28	33 duplicate
62	[812; D-Xylofuranose (4TMS)]		64 -0.696	0.890	9.653	0.630	18	123	22	119	42	23 original
99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]		64 -0.688	0.877	11.929	0.607	19	122	23	118	58	32 original
14	Fumaric acid		41 -0.685	0.953	8.740	0.655	20	121	6	135	35	7 original
28	Malic acid		64 -0.670	0.930	5.559	0.655	21	120	14	127	10	8 duplicate
40	[680; 2,3-Dimethylsuccinic acid (2TMS)]		64 -0.612	0.849	33.332	0.609	23	118	25	116	133	30 original
76	Fructose		64 -0.592	0.806	23.887	0.582	24	117	33	108	119	53 original
92	[680; Glycerol-2-phosphate (4TMS)]		54 -0.586	0.689	7.154	0.501	25	116	49	92	22	83 original
103	[648; Ethylamine (2TMS)]		63 -0.585	0.824	12.324	0.546	26	115	28	113	63	59 original
22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]		52 -0.585	0.915	9.574	0.627	27	114	18	123	41	26 duplicate
73	[708; Glucose methoxyamine (5TMS)]		57 -0.584	0.757	8.266	0.502	28	113	38	103	29	82 original
105	[705; 2-Keogluconic acid (5TMS)]		48 -0.574	0.838	10.191	0.585	29	112	26	115	50	47 original
21	[878; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]		64 -0.563	0.806	14.631	0.561	30	111	32	109	78	54 duplicate
78	Mannose		62 -0.552	0.762	8.833	0.525	31	110	37	104	37	71 original
106	[733; Threitol (4TMS)]		62 -0.547	0.814	8.679	0.655	32	109	30	111	34	9 original
35	Pyroglutamic acid		64 -0.547	0.794	40.144	0.566	33	108	34	107	138	52 original
70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]		57 -0.540	0.559	17.058	0.406	34	107	60	81	92	126 original
125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]		64 -0.540	0.711	30.499	0.529	35	106	47	94	129	67 original
26	Citramalic acid		64 -0.539	0.807	14.566	0.545	36	105	31	110	77	60 duplicate
115	Glucose-6-phosphate		62 -0.535	0.776	23.045	0.596	37	104	36	105	117	39 original
100	[857; Mannitol (6TMS)]		64 -0.528	0.816	5.953	0.554	38	103	29	112	11	56 original

3610	29 Erythritol	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	0.523	0.740	19.214	0.550	39	102	43	98	102	57 original
3615	29 Erythritol	102	[904; Galactose methoxyamine (5TMS)]	64	0.506	0.745	3.031	0.537	40	101	39	102	2	63 original
3641	29 Erythritol	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.499	0.838	6.159	0.566	41	100	27	114	15	51 original
3614	29 Erythritol	101	[832; Dopamine (4TMS)]	64	0.495	0.725	8.750	0.509	42	99	44	97	38	79 original
3633	29 Erythritol	120	[945; Uridine (3TMS)]	54	0.494	0.419	9.773	0.661	43	98	66	75	45	4 original
3625	29 Erythritol	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.493	0.743	13.975	0.543	44	97	40	101	72	61 original
3630	29 Erythritol	117	[724; Glycerol (3TMS)]	56	0.460	0.741	6.551	0.597	45	96	42	99	18	38 original
3648	29 Erythritol	135	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	0.457	0.657	10.176	0.503	46	95	51	90	49	81 original
3634	29 Erythritol	121	[657; Erythritol (4TMS)]	55	0.453	0.693	11.760	0.556	47	94	48	93	57	55 original
3604	29 Erythritol	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	0.434	0.676	15.590	0.479	48	93	50	91	81	91 original
3635	29 Erythritol	122	[644; Erythritol (4TMS)]	52	0.433	0.790	13.688	0.599	49	92	35	106	69	37 original
3623	29 Erythritol	110	[715; Erythritol (4TMS)]	54	0.433	0.742	10.392	0.636	50	91	41	100	51	19 original
10656	29 Erythritol	6	Glycerol	64	0.407	0.595	40.718	0.448	51	90	55	88	140	109 duplicate
3598	29 Erythritol	85	[528; Methylenic acid (4TMS)]	48	0.401	0.713	2.080	0.525	52	89	45	96	1	72 original
9971	29 Erythritol	1	[938; Sulfuric acid (2TMS)]	36	0.397	0.570	7.259	0.604	53	88	59	82	24	36 duplicate
3557	29 Erythritol	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	0.391	0.713	8.398	0.582	54	87	46	95	30	48 original
12198	29 Erythritol	18	[590; 1-Acetyl-2-thiohydantoin]	64	0.379	0.575	5.141	0.460	55	86	58	83	8	100 duplicate
3600	29 Erythritol	87	[945; beta-D-Glucopyranose (5TMS)]	62	0.373	0.587	34.024	0.458	56	85	57	84	136	103 original
3626	29 Erythritol	113	Galactose-6-phosphate	62	0.347	0.650	6.577	0.500	57	84	52	89	17	84 original
3645	29 Erythritol	132	[895; Isomaltose methoxyamine (8TMS)]	42	0.345	0.867	13.913	0.589	58	83	24	117	71	44 original
3640	29 Erythritol	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.317	0.645	4.126	0.593	59	82	53	88	5	41 original
3639	29 Erythritol	126	[559; Erythritol (4TMS)]	45	0.305	0.525	7.081	0.639	60	81	62	79	21	18 original
3587	29 Erythritol	116	[882; Pseudouridine (5TMS)]	30	0.301	0.501	7.470	0.317	61	80	64	77	25	139 original
3629	29 Erythritol	74	[912; Tetradecanoic acid (1TMS)]	64	0.285	0.549	8.544	0.526	62	79	61	80	32	69 original
3597	29 Erythritol	114	Fructose-6-phosphate	53	0.267	0.617	6.910	0.513	63	78	54	87	19	76 original
12320	29 Erythritol	64	Mannitol	62	0.263	0.588	30.319	0.498	64	77	56	85	127	86 original
3596	29 Erythritol	19	Alanine (BP) (3TMS)	64	0.254	0.507	10.070	0.470	65	76	63	78	47	95 duplicate
3617	29 Erythritol	83	Sorbitol	58	0.247	-0.354	20.594	0.423	66	75	93	48	110	119 original
3609	29 Erythritol	104	[795; Erythritol (4TMS)]	63	0.230	0.384	6.149	0.461	67	74	68	73	14	89 original
3606	29 Erythritol	96	myo-Inositol	49	0.214	0.213	16.770	0.294	68	73	78	65	90	140 original
3554	29 Erythritol	93	[607; Putrescine (4TMS)]	60	0.202	0.363	14.320	0.395	69	72	69	72	75	128 original
3593	29 Erythritol	41	[639; Proline (2TMS)]	64	0.174	0.345	12.006	0.442	70	71	70	71	60	111 original
3636	29 Erythritol	80	[772; D-Glucose (5TMS)]	62	0.173	0.446	29.499	0.416	71	70	65	76	124	122 original
3577	29 Erythritol	123	[945; Galactoturanose-6-phosphate (7TMS)]	64	0.165	0.313	8.946	0.460	72	69	72	69	40	101 original
11826	29 Erythritol	64	[789; Tyramine (3TMS)]	63	0.141	0.215	3.376	0.435	73	68	75	66	4	115 original
3624	29 Erythritol	15	Alanine	64	0.118	0.191	17.213	0.581	74	67	77	64	93	49 duplicate
3560	29 Erythritol	111	[583; Erythritol (4TMS)]	42	0.113	0.314	18.190	0.422	75	68	71	70	98	120 original
3592	29 Erythritol	47	[NA]	64	0.099	0.131	10.157	0.480	76	65	79	62	48	90 original
3566	29 Erythritol	79	Glucose	64	0.067	0.403	33.827	0.512	77	64	67	74	134	78 original
3646	29 Erythritol	53	Glycerol-2-phosphate	64	0.052	-0.018	8.602	0.408	78	63	83	58	33	124 original
3622	29 Erythritol	133	[855; Squalene]	64	0.052	-0.047	7.220	0.411	79	63	84	57	23	123 original
3653	29 Erythritol	109	Octadecanoic acid	64	0.030	0.304	21.342	0.459	80	61	73	68	112	102 original
3603	29 Erythritol	140	[682; Ergosta-7,22-dien-3-ol (1TMS)]	49	0.029	0.181	13.141	0.441	81	60	78	63	65	112 original
3607	29 Erythritol	90	[910; 9-(Z)-Hexadecanoic acid (1TMS)]	64	0.016	0.038	5.973	0.393	82	59	81	60	12	134 original
3576	29 Erythritol	94	Hexadecanoic acid	64	-0.015	0.220	20.486	0.472	83	58	74	67	109	93 original
3577	29 Erythritol	63	Glutamine	52	-0.053	-0.610	16.468	0.622	84	57	110	31	89	28 original
3584	29 Erythritol	71	[731; Erythrose (3TMS)]	64	-0.064	-0.205	10.539	0.432	85	56	88	53	53	116 original
3631	29 Erythritol	141	Lanosta-8,24-dien-3-beta-ol	61	-0.069	0.073	11.763	0.463	86	55	80	61	56	98 original
3650	29 Erythritol	118	[928; Glucopyranose-6-phosphate (6TMS)]	58	-0.122	-0.012	8.445	0.391	87	54	82	59	31	130 original
		137	Ergosterol	64	-0.128	-0.152	13.825	0.406	88		87	54	70	125 original

3620	29 Erythritol	107 9-(Z)-Octadecenoic acid	64 -0.129	-0.222	13.306	0.390	89	52	89	52	68	132 original
3565	29 Erythritol	52 [NA]	46 -0.130	-0.511	18.868	0.589	90	51	88	42	100	43 original
3632	29 Erythritol	119 [831; myc-Inositol-2-phosphate (7TMS)]	64 -0.135	-0.087	7.508	0.420	91	50	86	55	28	121 original
3551	29 Erythritol	138 [874; Ergosterol (1TMS)]	46 -0.144	-0.062	14.354	0.438	92	49	85	58	76	113 original
3652	29 Erythritol	139 [700; Ergosta-5,7-dien-3-ol]	38 -0.169	-0.224	16.132	0.345	93	48	90	51	87	138 original
3585	29 Erythritol	72 [918; D-Xylopyranose (4TMS)]	63 -0.179	-0.257	8.851	0.370	94	47	91	50	38	136 original
3611	29 Erythritol	98 [897; Ribose-5-phosphate methoxyamine (5TMS)]	48 -0.216	-0.739	17.618	0.586	95	46	124	17	95	40 original
3581	29 Erythritol	68 [570; Hypoxanthine (2TMS)]	20 -0.221	-0.883	13.382	0.509	96	45	137	4	88	80 original
3574	29 Erythritol	61 [NA]	64 -0.228	-0.292	5.342	0.424	97	44	92	49	9	117 original
3637	29 Erythritol	124 [734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecyloxyglycerol (1TMS)]	59 -0.229	-0.380	21.441	0.437	98	43	94	47	113	114 original
3602	29 Erythritol	89 [775; Dopamine (4TMS)]	35 -0.261	-0.707	16.350	0.454	99	42	118	23	88	107 original
10385	29 Erythritol	4 Phosphoric acid	51 -0.266	-0.526	33.041	0.346	100	41	101	40	132	137 duplicate
3556	29 Erythritol	43 [548; Leucine (2TBS)]	60 -0.267	-0.453	7.638	0.449	101	40	97	44	27	108 original
3543	29 Erythritol	130 Trehalose	63 -0.269	-0.423	28.901	0.382	102	39	95	48	122	135 original
13031	29 Erythritol	25 [709; 2,5-Diaminovalerolactam (2TMS)]	48 -0.270	-0.877	16.006	0.652	103	38	136	5	85	12 duplicate
10790	29 Erythritol	7 Threonine	64 -0.281	-0.552	29.307	0.446	104	37	102	39	123	110 duplicate
3649	29 Erythritol	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17 -0.309	-0.442	3.316	0.388	105	38	96	45	3	133 original
12788	29 Erythritol	23 Homoserine	64 -0.311	-0.849	12.138	0.625	106	35	133	8	61	27 duplicate
3621	29 Erythritol	108 Octadecenoic acid	64 -0.318	-0.496	7.056	0.384	107	34	98	43	20	129 original
3571	29 Erythritol	58 [636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64 -0.342	-0.514	15.772	0.424	108	33	100	41	84	118 original
13260	29 Erythritol	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53 -0.354	-0.851	18.681	0.605	109	32	134	7	99	34 duplicate
3579	29 Erythritol	66 Glycic acid-3-phosphate	64 -0.355	-0.645	6.076	0.519	110	31	115	26	13	73 original
10923	29 Erythritol	8 Isoleucine	55 -0.356	-0.602	19.359	0.390	111	30	108	33	103	131 duplicate
3558	29 Erythritol	45 Homocysteine	61 -0.360	-0.552	19.636	0.474	112	29	103	38	108	92 original
3549	29 Erythritol	36 [596; N-Acetylglutamic acid (2TMS)]	64 -0.368	-0.616	28.116	0.457	113	28	111	30	120	105 original
3588	29 Erythritol	75 Lysine	64 -0.371	-0.622	39.041	0.458	114	27	112	29	137	104 original
3580	29 Erythritol	67 Citric acid	64 -0.379	-0.553	22.735	0.403	115	26	104	37	116	127 original
3550	29 Erythritol	37 Phenylalanine	64 -0.388	-0.658	21.811	0.468	116	25	116	25	114	98 original
3573	29 Erythritol	60 Glycerol-3-phosphate	64 -0.397	-0.568	20.597	0.466	117	24	106	35	111	97 original
3544	29 Erythritol	31 [622; Parabanic acid (2TMS)]	64 -0.399	-0.722	9.965	0.537	118	23	121	20	46	62 original
3608	29 Erythritol	95 [770; 3,4,6-Trisubstitutedphenylmethanolamine (5TMS)]	50 -0.401	-0.586	17.737	0.456	119	22	107	34	98	106 original
3568	29 Erythritol	55 [612; 4-Aminobutyric acid (2TBS)]	43 -0.404	-0.639	19.582	0.471	120	21	114	27	105	94 original
3561	29 Erythritol	48 Asparagine	64 -0.405	-0.744	13.010	0.608	121	20	125	16	64	31 original
10110	29 Erythritol	2 Serine	62 -0.407	-0.687	18.820	0.490	122	19	117	24	107	87 duplicate
3547	29 Erythritol	34 Aspartic acid	64 -0.422	-0.624	32.294	0.512	123	18	113	28	131	77 original
3562	29 Erythritol	49 [877; Pyrophosphoric acid (4TMS)]	84 -0.424	-0.553	19.453	0.499	124	17	105	38	104	85 original
3644	29 Erythritol	131 [626; 5-Methylthioadenosine (3TMS)]	55 -0.444	-0.606	14.730	0.527	125	16	109	32	79	68 original
11055	29 Erythritol	9 Proline	63 -0.444	-0.713	28.177	0.481	126	15	119	22	121	89 duplicate
3564	29 Erythritol	51 [489; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44 -0.455	-0.780	17.574	0.535	127	14	128	13	94	65 original
3546	29 Erythritol	33 Methionine	64 -0.482	-0.713	11.959	0.534	128	13	120	21	59	66 original
10521	29 Erythritol	5 Leucine	45 -0.509	-0.844	10.511	0.588	129	12	132	9	52	45 duplicate
3543	29 Erythritol	30 [815; Ethyl-3(2H)-thiophenone]	64 -0.512	-0.723	29.785	0.483	130	11	122	19	125	88 original
10248	29 Erythritol	3 Ethanamine	62 -0.528	-0.761	11.030	0.516	131	10	126	15	54	75 duplicate
3545	29 Erythritol	32 [729; N,N-Dimethyllysine methyl ester]	63 -0.552	-0.869	17.050	0.645	132	9	135	6	91	15 original
12441	29 Erythritol	20 [619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	31 -0.557	-0.771	13.320	0.546	133	8	127	14	67	58 duplicate
3582	29 Erythritol	69 Arginine	60 -0.569	-0.896	21.929	0.629	134	7	139	2	115	24 original
3572	29 Erythritol	59 Ornithine; Arginine	64 -0.577	-0.737	40.362	0.516	135	6	123	18	139	74 original

3590	29 Erythritol	77	[826; beta-[[[5-methyl-2-thienyl)methyl]eneamino- benzeneacetic acid methyl ester]	-0.808	30,093	0.526	136	5	129	12	126	70 original
11186	29 Erythritol	10	Glycine	-0.593	19,076	0.629	137	4	138	3	101	25 duplicate
3594	29 Erythritol	81	Tyrosine	-0.614	33,967	0.604	138	3	131	10	135	35 original
3595	29 Erythritol	82	Lysine	-0.833	17,945	0.591	139	2	140	1	97	42 original
3555	29 Erythritol	42	Glutamic acid	-0.655	30,422	0.537	140	1	130	11	128	64 original
3657	30 [815; Ethyl-3(2H)-thioph	33	Methionine	0.889	24,271	0.574	1	140	2	139	55	6 original
3658	30 [815; Ethyl-3(2H)-thioph	34	Aspartic acid	0.795	5,741	0.600	2	139	1	140	1	4 original
3666	30 [815; Ethyl-3(2H)-thioph	42	Glutamic acid	0.779	9,652	0.618	3	138	3	138	5	1 original
3693	30 [815; Ethyl-3(2H)-thioph	69	Arginine	0.763	8,895	0.552	4	137	6	135	13	9 original
10522	30 [815; Ethyl-3(2H)-thioph	5	Leucine	0.886	29,727	0.601	5	136	7	134	85	3 duplicate
3675	30 [815; Ethyl-3(2H)-thioph	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	0.732	83,242	0.524	6	135	9	132	136	2 original
11056	30 [815; Ethyl-3(2H)-thioph	9	Proline	0.731	11,070	0.511	7	134	12	129	11	19 duplicate
10924	30 [815; Ethyl-3(2H)-thioph	8	Isoleucine	0.719	6,006	0.534	8	133	31	110	27	14 duplicate
3692	30 [815; Ethyl-3(2H)-thioph	68	[570; Hypoxanthine (2TMS)]	0.716	28,590	0.429	9	132	20	121	80	61 original
3656	30 [815; Ethyl-3(2H)-thioph	32	[729; N,N-Dimethyllysine methyl ester]	0.714	33,674	0.568	10	131	5	136	109	7 original
3701	30 [815; Ethyl-3(2H)-thioph	77	[826; beta-[[[5-methyl-2-thienyl)methyl]eneamino- benzeneacetic acid methyl ester]	0.713	8,899	0.528	11	130	8	133	2	16 original
3705	30 [815; Ethyl-3(2H)-thioph	81	Tyrosine	0.713	8,873	0.496	12	129	16	125	4	22 original
3683	30 [815; Ethyl-3(2H)-thioph	59	Ornithine; Arginine	0.708	14,100	0.501	13	128	4	137	19	21 original
3681	30 [815; Ethyl-3(2H)-thioph	37	Phenylalanine	0.684	10,494	0.514	14	127	14	127	8	17 original
11187	30 [815; Ethyl-3(2H)-thioph	10	Glycine	0.677	13,312	0.447	15	126	19	122	16	48 duplicate
3689	30 [815; Ethyl-3(2H)-thioph	45	Homocysteine	0.643	45,782	0.482	16	125	25	116	139	28 original
3706	30 [815; Ethyl-3(2H)-thioph	82	Lysine	0.628	15,688	0.536	17	124	13	128	20	13 original
3655	30 [815; Ethyl-3(2H)-thioph	31	[622; Parabenic acid (2TMS)]	0.627	34,089	0.434	18	123	23	118	111	57 original
10111	30 [815; Ethyl-3(2H)-thioph	2	Serine	0.615	17,927	0.543	19	122	15	126	28	12 duplicate
10249	30 [815; Ethyl-3(2H)-thioph	3	Ethanolamine	0.607	6,664	0.447	20	121	22	119	108	47 duplicate
3678	30 [815; Ethyl-3(2H)-thioph	55	[612; 4-Aminobutyric acid (2TBS)]	0.597	44,167	0.564	21	120	34	107	138	8 original
3672	30 [815; Ethyl-3(2H)-thioph	48	Asparagine	0.581	6,007	0.245	22	119	30	111	67	62 original
12799	30 [815; Ethyl-3(2H)-thioph	23	Homoserine	0.572	6,999	0.258	23	118	21	120	63	32 duplicate
3713	30 [815; Ethyl-3(2H)-thioph	89	[775; Dopamine (4TMS)]	0.570	6,625	0.497	24	117	29	112	98	11 original
10791	30 [815; Ethyl-3(2H)-thioph	7	Threonine	0.564	8,782	0.512	25	116	11	130	3	18 duplicate
3691	30 [815; Ethyl-3(2H)-thioph	67	Citric acid	0.502	6,654	0.406	26	115	24	117	9	71 original
3685	30 [815; Ethyl-3(2H)-thioph	61	[NA]	0.498	4,235	0.365	27	114	36	105	73	108 original
3690	30 [815; Ethyl-3(2H)-thioph	66	Glycemic acid-3-phosphate	0.496	6,641	0.395	28	113	27	114	88	80 original
3684	30 [815; Ethyl-3(2H)-thioph	60	Glycerol-3-phosphate	0.484	6,601	0.426	29	112	33	108	12	64 original
3722	30 [815; Ethyl-3(2H)-thioph	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	0.466	6,603	0.418	30	111	32	109	130	29 original
3719	30 [815; Ethyl-3(2H)-thioph	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	0.466	4,211	0.416	31	110	38	103	134	65 original
13261	30 [815; Ethyl-3(2H)-thioph	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	0.462	8,800	0.550	32	109	10	131	126	10 duplicate
13032	30 [815; Ethyl-3(2H)-thioph	25	[709; 2,5-Diaminovalerolactam (2TMS)]	0.450	6,641	0.364	33	108	26	115	78	108 duplicate
12442	30 [815; Ethyl-3(2H)-thioph	20	[619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	0.445	33,834	0.581	34	107	28	113	110	5 duplicate
3755	30 [815; Ethyl-3(2H)-thioph	131	[626; 5-Methylthioadenosine (3TMS)]	0.436	39,006	0.391	35	106	45	96	129	85 original
3673	30 [815; Ethyl-3(2H)-thioph	49	[877; Pyrophosphoric acid (4TMS)]	0.412	42,501	0.369	36	105	44	97	135	102 original
3760	30 [815; Ethyl-3(2H)-thioph	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	0.382	12,370	0.317	37	104	35	106	14	132 original
3699	30 [815; Ethyl-3(2H)-thioph	75	Lysine	0.359	13,963	0.508	38	103	18	123	17	20 original
3676	30 [815; Ethyl-3(2H)-thioph	52	[NA]	0.333	37,105	0.475	39	102	46	95	124	28 original
3687	30 [815; Ethyl-3(2H)-thioph	43	[548; Leucine (2TBS)]	0.302	4,412	0.415	40	101	37	104	65	66 original
3682	30 [815; Ethyl-3(2H)-thioph	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	0.293	15,754	0.490	41	100	17	124	21	23 original
3732	30 [815; Ethyl-3(2H)-thioph	108	Octadecenoic acid	0.275	30,711	0.375	42	99	47	94	95	95 original

3695	30 [815; Ethyl-3(2H)-thioph	71	[731; Erythrose (3TMS)]	64	0.267	0.409	19.800	0.395	43	98	40	101	39	81	original
3687	30 [815; Ethyl-3(2H)-thioph	63	Glutamine	52	0.256	0.403	29.815	0.368	44	97	41	100	87	104	original
3660	30 [815; Ethyl-3(2H)-thioph	36	[596; N-Acetylglutamic acid (2TMS)]	64	0.203	0.398	10.371	0.459	45	98	42	99	7	33	original
3754	30 [815; Ethyl-3(2H)-thioph	130	Trehalose	63	0.137	0.293	10.684	0.364	46	95	48	93	10	107	original
3748	30 [815; Ethyl-3(2H)-thioph	124	[734; 1-Monodoleoylglycerol (2TMS); 1-Monohexadecenoylethanol (1TMS)]	59	0.126	0.207	47.024	0.352	47	94	50	91	140	119	original
10386	30 [815; Ethyl-3(2H)-thioph	4	Phosphoric acid	51	0.123	0.392	10.346	0.459	48	93	43	98	6	34	duplicate
3731	30 [815; Ethyl-3(2H)-thioph	107	[9-Z]-Octadecenoic acid	64	0.087	0.128	18.164	0.341	49	92	52	89	30	125	original
11827	30 [815; Ethyl-3(2H)-thioph	15	Alanine	64	0.084	0.038	17.000	0.466	50	91	56	85	25	30	duplicate
3743	30 [815; Ethyl-3(2H)-thioph	119	[931; myo-Inositol-2-phosphate (7TMS)]	64	0.048	-0.033	27.007	0.370	51	90	58	83	70	101	original
3763	30 [815; Ethyl-3(2H)-thioph	139	[700; Ergosta-5,7-dien-3-ol]	38	0.041	0.237	35.787	0.272	52	89	49	92	118	138	original
3761	30 [815; Ethyl-3(2H)-thioph	137	Ergosterol	64	0.037	0.137	21.765	0.372	53	88	51	90	51	98	original
3688	30 [815; Ethyl-3(2H)-thioph	64	[789; Tyramine (3TMS)]	63	0.024	0.101	28.982	0.334	54	87	53	88	82	127	original
3707	30 [815; Ethyl-3(2H)-thioph	83	Sorbitol	58	0.007	0.409	13.180	0.446	55	86	39	102	15	50	original
3735	30 [815; Ethyl-3(2H)-thioph	111	[583; Erythritol (4TMS)]	42	-0.008	-0.047	38.317	0.282	56	85	59	82	127	137	original
3762	30 [815; Ethyl-3(2H)-thioph	138	[674; Ergosterol (1TMS)]	46	-0.020	0.047	36.076	0.299	57	84	55	86	119	134	original
3714	30 [815; Ethyl-3(2H)-thioph	90	[910; 9-Z]-Hexadecenoic acid (1TMS)]	64	-0.022	-0.103	26.627	0.333	58	83	63	78	69	128	original
3717	30 [815; Ethyl-3(2H)-thioph	93	[607; Putrescine (4TMS)]	60	-0.032	-0.227	40.504	0.358	59	82	70	71	131	115	original
3677	30 [815; Ethyl-3(2H)-thioph	53	Glycerol-2-phosphate	64	-0.058	-0.138	36.015	0.357	60	81	65	78	118	117	original
3696	30 [815; Ethyl-3(2H)-thioph	72	[919; D-Xylopyranose (4TMS)]	63	-0.061	0.002	32.065	0.358	61	80	57	84	100	116	original
3718	30 [815; Ethyl-3(2H)-thioph	94	Hexadecanoic acid	64	-0.066	-0.098	16.552	0.380	62	79	62	78	24	92	original
3703	30 [815; Ethyl-3(2H)-thioph	79	Glucose	64	-0.079	-0.238	16.514	0.391	63	78	71	70	23	84	original
3757	30 [815; Ethyl-3(2H)-thioph	133	[855; Squalene]	64	-0.085	0.087	27.500	0.378	64	77	54	87	74	93	original
3765	30 [815; Ethyl-3(2H)-thioph	141	[Lanosta-8,24-dien-3-beta-ol]	61	-0.091	-0.198	38.861	0.404	65	76	68	73	128	72	original
3751	30 [815; Ethyl-3(2H)-thioph	127	[777; Fructose-6-phosphate methoxamine (6TMS)]	39	-0.093	-0.305	19.687	0.176	66	75	76	65	38	140	original
3733	30 [815; Ethyl-3(2H)-thioph	109	Octadecanoic acid	64	-0.093	-0.163	20.529	0.359	67	74	68	75	45	114	original
3742	30 [815; Ethyl-3(2H)-thioph	118	[928; Glucopyranose-6-phosphate (6TMS)]	58	-0.129	-0.061	30.243	0.322	68	73	60	81	92	131	original
3720	30 [815; Ethyl-3(2H)-thioph	96	myo-Inositol	49	-0.155	-0.122	42.093	0.361	69	72	64	77	133	112	original
3740	30 [815; Ethyl-3(2H)-thioph	116	[882; Pseudouridine (5TMS)]	30	-0.172	-0.273	24.728	0.390	70	71	73	68	60	86	original
3708	30 [815; Ethyl-3(2H)-thioph	84	Mannitol	62	-0.175	-0.536	20.034	0.450	71	70	102	39	41	44	original
3747	30 [815; Ethyl-3(2H)-thioph	123	[945; Galactofuranose-6-phosphate (7TMS)]	64	-0.183	-0.085	22.297	0.398	72	69	61	80	52	78	original
3759	30 [815; Ethyl-3(2H)-thioph	140	[902; Melibiose (6TMS); alpha-D-Gal-(1,6)-D-Glc (6TMS)]	64	-0.186	-0.290	20.323	0.347	73	68	75	66	43	121	original
3764	30 [815; Ethyl-3(2H)-thioph	132	[892; Ergosta-7,22-dien-3-ol (1TMS)]	49	-0.192	-0.221	37.836	0.350	74	67	69	72	125	120	original
3756	30 [815; Ethyl-3(2H)-thioph	132	[895; Isomaltose methoxamine (6TMS)]	42	-0.231	-0.584	33.011	0.284	75	66	108	33	105	136	original
3738	30 [815; Ethyl-3(2H)-thioph	114	Fructose-6-phosphate	53	-0.232	-0.327	30.331	0.341	76	65	78	63	93	124	original
3726	30 [815; Ethyl-3(2H)-thioph	102	[904; Galactose methoxamine (5TMS)]	64	-0.258	-0.398	31.363	0.360	77	64	83	58	88	113	original
3737	30 [815; Ethyl-3(2H)-thioph	113	Galactose-6-phosphate	62	-0.262	-0.372	32.696	0.384	78	63	81	60	103	89	original
3671	30 [815; Ethyl-3(2H)-thioph	47	[NA]	64	-0.264	-0.277	30.349	0.400	79	62	74	67	94	76	original
3736	30 [815; Ethyl-3(2H)-thioph	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	-0.276	-0.410	41.842	0.362	80	61	85	56	132	110	original
3750	30 [815; Ethyl-3(2H)-thioph	126	[559; Erythritol (4TMS)]	45	-0.277	-0.254	25.217	0.334	81	60	72	69	64	128	original
3752	30 [815; Ethyl-3(2H)-thioph	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	-0.301	-0.494	20.952	0.296	82	59	52	48	135	original	
3709	30 [815; Ethyl-3(2H)-thioph	85	[529; Methylcitrinic acid (4TMS)]	48	-0.307	-0.495	27.312	0.533	83	58	96	45	72	15	original
9972	30 [815; Ethyl-3(2H)-thioph	1	[938; Sulfuric acid (2TMS)]	36	-0.308	-0.486	21.202	0.250	84	57	94	47	49	139	duplicate
3728	30 [815; Ethyl-3(2H)-thioph	104	[795; Erythritol (4TMS)]	63	-0.310	-0.344	28.396	0.441	85	56	79	62	84	53	original
3724	30 [815; Ethyl-3(2H)-thioph	100	[857; Mannitol (6TMS)]	64	-0.321	-0.529	24.921	0.378	86	55	100	41	62	94	original
3698	30 [815; Ethyl-3(2H)-thioph	74	[912; Tetradecanoic acid (1TMS)]	64	-0.348	-0.371	32.773	0.449	87	54	80	61	104	45	original
3665	30 [815; Ethyl-3(2H)-thioph	41	[639; Proline (2TMS)]	64	-0.350	-0.195	20.362	0.393	88	53	67	74	44	82	original
3659	30 [815; Ethyl-3(2H)-thioph	35	Pyrogutamic acid	64	-0.372	-0.471	19.448	0.370	89	52	91	50	35	100	original
12199	30 [815; Ethyl-3(2H)-thioph	18	[590; 1-Acetyl-2-thiohydantoin]	64	-0.373	-0.404	26.070	0.380	90	51	84	57	66	91	duplicate
10657	30 [815; Ethyl-3(2H)-thioph	6	Glycerol	64	-0.375	-0.463	19.409	0.387	91	50	90	51	34	87	duplicate

12321	30 [815; Ethyl-3(2H)-thioph	19	Alanine (BP) (3TMS)	64 -0.387	-0.313	23.276	0.363	92	49	77	64	53	109 duplicate
3744	30 [815; Ethyl-3(2H)-thioph	120	[945; Uridine (3TMS)]	54 -0.398	-0.424	19.509	0.402	93	48	88	53	36	73 original
3704	30 [815; Ethyl-3(2H)-thioph	80	[772; D-Glucose (5TMS)]	62 -0.411	-0.418	19.345	0.346	94	47	87	54	33	122 original
3668	30 [815; Ethyl-3(2H)-thioph	44	[910; 2-Keitoglucosidic acid methoxyamine (4TMS)]	50 -0.412	-0.487	24.740	0.327	95	46	95	46	61	129 original
3715	30 [815; Ethyl-3(2H)-thioph	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64 -0.416	-0.580	33.578	0.408	96	45	108	35	107	70 original
11446	30 [815; Ethyl-3(2H)-thioph	12	Glyceric acid	63 -0.425	-0.678	36.692	0.415	97	44	124	17	121	67 duplicate
3739	30 [815; Ethyl-3(2H)-thioph	115	Glucose-6-phosphate	62 -0.434	-0.502	16.226	0.384	98	43	97	44	22	88 original
3697	30 [815; Ethyl-3(2H)-thioph	73	[708; Glucose methoxyamine (5TMS)]	57 -0.435	-0.391	33.488	0.448	99	42	82	59	106	46 original
13374	30 [815; Ethyl-3(2H)-thioph	28	Malic acid	64 -0.439	-0.652	24.432	0.455	100	41	119	22	58	40 duplicate
3721	30 [815; Ethyl-3(2H)-thioph	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52 -0.442	-0.597	24.416	0.368	101	40	110	31	57	105 original
3725	30 [815; Ethyl-3(2H)-thioph	101	[832; Dopamine (4TMS)]	64 -0.465	-0.583	30.238	0.431	102	39	107	34	91	58 original
3745	30 [815; Ethyl-3(2H)-thioph	121	[657; Erythritol (4TMS)]	55 -0.472	-0.482	36.578	0.361	103	38	93	48	120	111 original
3723	30 [815; Ethyl-3(2H)-thioph	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41 -0.476	-0.640	27.817	0.323	104	37	116	25	77	130 original
13147	30 [815; Ethyl-3(2H)-thioph	26	Citramalic acid	64 -0.481	-0.547	17.172	0.410	105	36	104	37	28	68 duplicate
3749	30 [815; Ethyl-3(2H)-thioph	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64 -0.486	-0.512	19.544	0.399	106	35	98	43	37	77 original
3678	30 [815; Ethyl-3(2H)-thioph	54	[NA]	55 -0.494	-0.600	34.453	0.344	107	34	111	30	112	123 original
3716	30 [815; Ethyl-3(2H)-thioph	92	[680; Glycerol-2-phosphate (4TMS)]	54 -0.494	-0.481	28.201	0.314	108	33	92	49	79	133 original
11317	30 [815; Ethyl-3(2H)-thioph	11	Succinic acid	64 -0.495	-0.629	26.331	0.452	109	32	114	27	68	42 duplicate
3734	30 [815; Ethyl-3(2H)-thioph	110	[715; Erythritol (4TMS)]	54 -0.497	-0.530	32.484	0.409	110	31	101	40	102	69 original
3746	30 [815; Ethyl-3(2H)-thioph	122	[644; Erythritol (4TMS)]	52 -0.501	-0.560	36.841	0.353	111	30	105	36	122	118 original
3741	30 [815; Ethyl-3(2H)-thioph	117	[724; Glycerol (3TMS)]	56 -0.508	-0.547	30.009	0.372	112	29	103	38	89	97 original
11701	30 [815; Ethyl-3(2H)-thioph	14	Fumaric acid	64 -0.511	-0.681	34.845	0.453	113	28	125	16	113	41 duplicate
13486	30 [815; Ethyl-3(2H)-thioph	29	Erythritol	64 -0.512	-0.723	29.785	0.483	114	27	133	8	86	24 duplicate
12681	30 [815; Ethyl-3(2H)-thioph	22	[690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	52 -0.517	-0.675	35.991	0.478	115	28	123	18	117	27 duplicate
3729	30 [815; Ethyl-3(2H)-thioph	105	[705; 2-Keitoglucosidic acid (5TMS)]	48 -0.520	-0.655	24.398	0.367	116	25	120	21	56	103 original
3727	30 [815; Ethyl-3(2H)-thioph	103	[648; Ethylamine (2TMS)]	63 -0.520	-0.642	30.816	0.427	117	24	117	24	97	63 original
3700	30 [815; Ethyl-3(2H)-thioph	76	Fructose	64 -0.521	-0.587	20.694	0.382	118	23	109	32	48	90 original
3664	30 [815; Ethyl-3(2H)-thioph	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64 -0.527	-0.640	13.986	0.456	119	22	115	26	18	39 original
3680	30 [815; Ethyl-3(2H)-thioph	56	[828; Oxalic acid (3TMS)]	64 -0.528	-0.673	35.742	0.442	120	21	122	19	115	51 original
3662	30 [815; Ethyl-3(2H)-thioph	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64 -0.534	-0.732	27.309	0.442	121	20	135	6	71	52 original
12562	30 [815; Ethyl-3(2H)-thioph	81	[678; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	64 -0.538	-0.684	16.758	0.439	122	19	126	15	32	54 duplicate
3711	30 [815; Ethyl-3(2H)-thioph	87	[945; beta-D-Glucopyranose (5TMS)]	62 -0.542	-0.526	20.870	0.372	123	18	99	42	47	99 original
3702	30 [815; Ethyl-3(2H)-thioph	78	Mannose	62 -0.544	-0.643	35.343	0.400	124	17	118	23	114	74 original
3694	30 [815; Ethyl-3(2H)-thioph	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57 -0.555	-0.415	17.937	0.400	125	16	86	55	29	75 original
12076	30 [815; Ethyl-3(2H)-thioph	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64 -0.563	-0.690	21.233	0.457	126	15	127	14	50	37 duplicate
3681	30 [815; Ethyl-3(2H)-thioph	57	[757; 2-Desoxy-pentose-3-ylose dimethoxyamine (2TMS)]	55 -0.566	-0.661	28.709	0.373	127	14	121	20	81	96 original
12916	30 [815; Ethyl-3(2H)-thioph	24	[725; 2-Ketobutanoic acid (2TMS)]	64 -0.568	-0.750	18.212	0.457	128	13	137	4	31	38 duplicate
11952	30 [815; Ethyl-3(2H)-thioph	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64 -0.570	-0.756	20.028	0.483	129	12	138	3	40	25 duplicate
3712	30 [815; Ethyl-3(2H)-thioph	88	Glucosidic acid	64 -0.581	-0.695	27.559	0.458	130	11	128	13	75	35 original
3730	30 [815; Ethyl-3(2H)-thioph	108	[733; Threitol (4TMS)]	62 -0.583	-0.610	29.096	0.447	131	10	112	29	83	49 original
3686	30 [815; Ethyl-3(2H)-thioph	62	[812; D-Xylofuranose (4TMS)]	64 -0.583	-0.610	20.149	0.391	132	9	113	28	42	83 original
3758	30 [815; Ethyl-3(2H)-thioph	134	Isomaltose	64 -0.592	-0.724	24.595	0.435	133	8	134	7	59	55 original
3663	30 [815; Ethyl-3(2H)-thioph	39	[829; 1-Phenylethanol (1TMS)]	63 -0.608	-0.744	27.696	0.429	134	7	136	5	76	59 original
3670	30 [815; Ethyl-3(2H)-thioph	46	Arabinose	64 -0.613	-0.708	30.092	0.435	135	6	130	11	90	58 original
3710	30 [815; Ethyl-3(2H)-thioph	86	[793; D-Galactono-1,4-lactone (4TMS)]	61 -0.614	-0.697	30.722	0.452	136	5	129	12	96	43 original
3689	30 [815; Ethyl-3(2H)-thioph	65	[646; 3-Deoxyglucitol (5TMS)]	63 -0.619	-0.719	36.880	0.429	137	4	132	9	123	60 original
3753	30 [815; Ethyl-3(2H)-thioph	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59 -0.627	-0.710	32.321	0.396	138	3	131	10	101	79 original
11574	30 [815; Ethyl-3(2H)-thioph	13	Uracil	64 -0.632	-0.757	23.429	0.465	139	2	139	2	54	31 duplicate
3674	30 [815; Ethyl-3(2H)-thioph	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61 -0.685	-0.777	44.026	0.457	140	1	140	1	137	36 original

11057	31 [622; Parabanic acid (21 9	Proline	63	0.747	0.763	30.371	0.478	1	140	8	133	117	57 duplicate
10925	31 [622; Parabanic acid (21 8	Isoleucine	55	0.717	0.707	20.111	0.451	2	139	17	124	93	76 duplicate
3802	31 [622; Parabanic acid (21 68	[570; Hypoxanthine (2TMS)]	20	0.705	0.734	10.274	0.476	3	138	14	127	23	58 original
12800	31 [622; Parabanic acid (21 23	Homoserine	64	0.666	0.836	10.781	0.561	4	137	1	140	28	3 duplicate
10112	31 [622; Parabanic acid (21 2	Serine	62	0.662	0.743	20.694	0.463	5	138	11	130	94	68 duplicate
3767	31 [622; Parabanic acid (21 33	Methionine	64	0.645	0.635	11.581	0.519	6	135	25	118	39	32 original
13598	31 [622; Parabanic acid (21 30	[815; Ethyl-3(2H)-thiophenone]	64	0.627	0.660	34.089	0.434	7	134	21	120	124	90 duplicate
3800	31 [622; Parabanic acid (21 66	Glycine acid-3-phosphate	64	0.613	0.761	5.629	0.532	8	133	9	132	2	25 original
3766	31 [622; Parabanic acid (21 32	[729; N,N-Dimethyllysine methyl ester]	63	0.609	0.779	9.764	0.536	9	132	5	136	18	17 original
3793	31 [622; Parabanic acid (21 59	Ornithine; Arginine	64	0.603	0.736	46.011	0.504	10	131	13	128	138	38 original
11188	31 [622; Parabanic acid (21 10	Glycine	64	0.583	0.766	22.737	0.533	11	130	7	134	99	23 duplicate
3815	31 [622; Parabanic acid (21 81	Tyrosine	64	0.568	0.739	38.347	0.500	12	129	12	129	132	42 original
10792	31 [622; Parabanic acid (21 7	Threonine	64	0.564	0.688	35.329	0.450	13	128	18	123	126	78 duplicate
13262	31 [622; Parabanic acid (21 27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	0.559	0.790	12.094	0.550	14	127	4	137	42	6 duplicate
3803	31 [622; Parabanic acid (21 69	Arginine	60	0.558	0.775	23.874	0.550	15	126	6	135	105	5 original
3768	31 [622; Parabanic acid (21 34	Aspartic acid	64	0.547	0.596	37.621	0.485	16	125	27	114	129	49 original
3776	31 [622; Parabanic acid (21 42	Glutamic acid	60	0.540	0.749	32.387	0.495	17	124	10	131	120	43 original
3782	31 [622; Parabanic acid (21 48	Asparagine	64	0.534	0.684	11.609	0.500	18	123	20	121	40	41 original
3811	31 [622; Parabanic acid (21	[826; beta-[[[5-methyl-2-thienyl)methyleneamino-benzeneacetic acid methyl ester]	62	0.534	0.727	33.335	0.452	19	122	15	126	122	75 original
3771	31 [622; Parabanic acid (21 37	Phenylalanine	64	0.531	0.718	27.747	0.465	20	121	16	125	112	86 original
10250	31 [622; Parabanic acid (21 3	Ethanolamine	62	0.504	0.855	5.195	0.439	21	120	22	119	1	85 duplicate
3785	31 [622; Parabanic acid (21 51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	0.503	0.819	13.445	0.535	22	119	2	139	59	19 original
3832	31 [622; Parabanic acid (21 98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	48	0.500	0.689	11.161	0.503	23	118	19	122	32	40 original
13033	31 [622; Parabanic acid (21 25	[708; 2,5-Diaminovalerolactam (2TMS)]	48	0.468	0.794	9.507	0.519	24	117	3	138	16	30 duplicate
10523	31 [622; Parabanic acid (21 5	Leucine	45	0.465	0.630	6.949	0.567	25	116	26	115	6	1 duplicate
3779	31 [622; Parabanic acid (21 45	Homocysteine	61	0.445	0.480	13.440	0.480	26	115	35	108	58	53 original
3809	31 [622; Parabanic acid (21 75	Lysine	64	0.437	0.654	44.827	0.434	27	114	23	118	137	89 original
3823	31 [622; Parabanic acid (21 89	[775; Dopamine (4TMS)]	35	0.435	0.523	12.420	0.412	28	113	32	109	45	103 original
3784	31 [622; Parabanic acid (21	Glycerol-3-phosphate	64	0.399	0.555	26.337	0.438	29	112	31	110	110	86 original
3792	31 [622; Parabanic acid (21	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	0.386	0.575	20.048	0.436	30	111	28	112	92	87 original
3801	31 [622; Parabanic acid (21 67	Clitic acid	64	0.383	0.566	28.983	0.371	31	110	30	111	116	125 original
3816	31 [622; Parabanic acid (21 82	Lysine	39	0.360	0.637	17.502	0.545	32	109	24	117	81	8 original
3777	31 [622; Parabanic acid (21 43	[548; Leucine (2TBS)]	60	0.356	0.492	10.475	0.393	33	108	33	108	25	113 original
3865	31 [622; Parabanic acid (21 131	[626; 5-Methylthioadenosine (3TMS)]	55	0.352	0.481	8.774	0.409	34	107	34	107	12	104 original
3795	31 [622; Parabanic acid (21 61	[NA]	64	0.312	0.354	9.084	0.377	35	106	43	88	13	122 original
3770	31 [622; Parabanic acid (21 36	[596; N-Acetylglutamic acid (2TMS)]	64	0.311	0.594	33.476	0.483	36	105	28	113	123	52 original
3789	31 [622; Parabanic acid (21 55	[612; 4-Aminobutyric acid (2TBS)]	43	0.298	0.348	16.761	0.467	37	104	46	85	76	64 original
3786	31 [622; Parabanic acid (21 52	[NA]	46	0.287	0.361	13.220	0.460	38	103	41	100	55	70 original
3783	31 [622; Parabanic acid (21 49	[877; Pyrophosphoric acid (4TMS)]	64	0.267	0.361	13.305	0.388	39	102	42	99	57	115 original
3829	31 [622; Parabanic acid (21 95	[770; 3,4,6-Trisubstitutedphenylethandamine (5TMS)]	50	0.262	0.392	12.968	0.354	40	101	39	102	52	130 original
3870	31 [622; Parabanic acid (21 136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.235	0.395	6.334	0.381	41	100	38	103	3	119 original
3864	31 [622; Parabanic acid (21 130	Trehalose	63	0.230	0.350	35.257	0.378	42	99	45	96	125	121 original
3805	31 [622; Parabanic acid (21 71	[731; Erythrose (3TMS)]	64	0.199	0.353	16.811	0.456	43	98	44	97	77	71 original
3797	31 [622; Parabanic acid (21 63	Glutamine	52	0.199	0.411	13.094	0.479	44	97	37	104	53	55 original
3842	31 [622; Parabanic acid (21 108	Octadecenoic acid	64	0.186	0.317	7.117	0.383	45	96	48	93	7	117 original
12443	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	0.178	0.467	11.268	0.551	46	95	36	105	35	4 duplicate
10387	31 [622; Parabanic acid (21 4	Phosphoric acid	51	0.158	0.338	36.521	0.402	47	94	47	94	127	107 duplicate
11828	31 [622; Parabanic acid (21 15	Alanine	64	0.132	0.066	23.598	0.492	48	93	52	89	103	45 duplicate

3817	31 [622; Parabanic acid (21 83 Sorbitol	58	0,101	0,388	24,651	0,444	49	92	40	101	108	81 original
3798	31 [622; Parabanic acid (21 64 [789; Tyramine (3TMS)]	63	0,078	0,048	8,111	0,350	50	91	54	87	8	131 original
	124 [734; 1-Monooctadecanoylglycerol (1TMS)]											
3858	31 [622; Parabanic acid (21 Monohexadecanoylglycerol (1TMS)]	59	0,073	0,233	15,271	0,348	51	90	49	92	71	133 original
3813	31 [622; Parabanic acid (21 79 Glucose	64	0,036	-0,178	40,720	0,442	52	89	66	75	135	83 original
3871	31 [622; Parabanic acid (21 137 Ergosterol	64	-0,013	0,162	18,602	0,361	53	88	50	91	85	129 original
3845	31 [622; Parabanic acid (21 111 [583; Erythritol (4TMS)]	42	-0,022	-0,076	12,586	0,363	54	87	57	84	48	127 original
3867	31 [622; Parabanic acid (21 133 [855; Squalene]	64	-0,028	0,139	11,182	0,374	55	86	51	90	33	124 original
3872	31 [622; Parabanic acid (21 138 [674; Ergosterol (1TMS)]	46	-0,032	0,042	9,581	0,382	56	85	55	86	17	118 original
3841	31 [622; Parabanic acid (21 107 9-(Z)-Octadecenoic acid	64	-0,040	0,053	19,625	0,338	57	84	53	88	90	135 original
3787	31 [622; Parabanic acid (21 53 Glycerol-2-phosphate	64	-0,075	-0,052	6,362	0,320	58	83	56	85	5	138 original
3853	31 [622; Parabanic acid (21 119 [931; myo-Inositol-2-phosphate (7TMS)]	64	-0,079	-0,118	12,491	0,400	59	82	59	82	46	111 original
3857	31 [622; Parabanic acid (21 123 [945; Galactofuranose-6-phosphate (7TMS)]	64	-0,091	-0,117	15,884	0,448	60	81	58	83	75	79 original
3838	31 [622; Parabanic acid (21 104 [795; Erythritol (4TMS)]	63	-0,102	-0,136	11,458	0,403	61	80	60	81	37	108 original
3843	31 [622; Parabanic acid (21 109 Octadecanoic acid	64	-0,111	-0,158	27,929	0,348	62	79	63	78	113	132 original
3828	31 [622; Parabanic acid (21 94 Hexadecanoic acid	64	-0,118	-0,137	27,198	0,428	63	78	61	80	111	98 original
3806	31 [622; Parabanic acid (21 72 [919; D-Xylopyranose (4TMS)]	63	-0,121	-0,181	10,284	0,328	64	77	67	74	24	137 original
3852	31 [622; Parabanic acid (21 118 [928; Glucopyranose-6-phosphate (6TMS)]	58	-0,131	-0,191	10,507	0,312	65	76	68	73	26	139 original
3847	31 [622; Parabanic acid (21 113 Galactose-6-phosphate	62	-0,139	-0,356	10,878	0,397	66	75	75	66	29	112 original
3873	31 [622; Parabanic acid (21 139 [700; Ergosterol-5,7-dien-3-ol]	38	-0,144	-0,152	11,324	0,293	67	74	62	79	38	140 original
3875	31 [622; Parabanic acid (21 141 Lanosta-8,24-dien-3-beta-ol	61	-0,145	-0,170	9,398	0,393	68	73	64	77	14	114 original
3827	31 [622; Parabanic acid (21 93 [607; Putrescine (4TMS)]	60	-0,153	-0,337	12,507	0,368	69	72	71	70	47	126 original
3824	31 [622; Parabanic acid (21 90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	64	-0,159	-0,178	11,891	0,335	70	71	65	76	41	136 original
3830	31 [622; Parabanic acid (21 86 myo-Inositol	49	-0,162	-0,225	12,762	0,363	71	70	69	72	49	128 original
10658	31 [622; Parabanic acid (21 6 Glycerol	64	-0,173	-0,343	47,583	0,433	72	69	73	68	140	92 duplicate
3848	31 [622; Parabanic acid (21 114 Fructose-6-phosphate	53	-0,183	-0,384	9,777	0,402	73	68	79	62	19	108 original
3860	31 [622; Parabanic acid (21 126 [559; Erythritol (4TMS)]	45	-0,194	-0,307	10,662	0,495	74	67	70	71	27	44 original
3775	31 [622; Parabanic acid (21 41 [639; Proline (2TMS)]	64	-0,247	-0,357	19,278	0,431	75	66	76	65	89	96 original
12322	31 [622; Parabanic acid (21 19 Alanine (BP) (3TMS)	64	-0,248	-0,378	17,663	0,424	76	65	78	63	82	100 duplicate
3807	31 [622; Parabanic acid (21 73 [708; Glucose methoxamine (5TMS)]	57	-0,249	-0,343	12,416	0,435	77	64	72	69	44	88 original
3874	31 [622; Parabanic acid (21 140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49	-0,259	-0,360	9,828	0,430	78	63	77	64	20	97 original
3818	31 [622; Parabanic acid (21 84 Mannitol	62	-0,267	-0,662	37,946	0,491	79	62	115	26	130	46 original
3819	31 [622; Parabanic acid (21 85 [529; Methylcitric acid (4TMS)]	48	-0,268	-0,538	6,381	0,532	80	61	102	39	4	24 original
3769	31 [622; Parabanic acid (21 35 Pyroglutamic acid	64	-0,273	-0,498	47,226	0,433	81	60	92	49	139	93 original
3838	31 [622; Parabanic acid (21 102 [904; Galactose methoxamine (5TMS)]	64	-0,278	-0,401	8,277	0,453	82	59	82	59	10	73 original
3861	31 [622; Parabanic acid (21 127 [777; Fructose-6-phosphate methoxamine (6TMS)]	39	-0,285	-0,519	10,941	0,440	83	58	97	44	30	84 original
3778	31 [622; Parabanic acid (21 44 [910; 2-Ketogluconic acid methoxamine (4TMS)]	50	-0,285	-0,427	15,759	0,476	84	57	84	57	74	59 original
	135											
3869	31 [622; Parabanic acid (21 [902; Melibiose (6TMS); alpha-D-Gal-(1,8)-D-Glc (6TMS)]	64	-0,287	-0,455	17,387	0,451	85	56	88	53	80	77 original
3781	31 [622; Parabanic acid (21 47 [NA]	64	-0,290	-0,396	15,110	0,401	86	55	81	60	70	110 original
3855	31 [622; Parabanic acid (21 121 [657; Erythritol (4TMS)]	55	-0,296	-0,410	11,002	0,455	87	54	83	58	31	72 original
3814	31 [622; Parabanic acid (21 80 [772; D-Glucose (5TMS)]	62	-0,301	-0,476	36,842	0,380	88	53	90	51	128	120 original
3810	31 [622; Parabanic acid (21 76 Fructose	64	-0,305	-0,528	32,084	0,453	89	52	99	42	119	74 original
3844	31 [622; Parabanic acid (21 110 [715; Erythritol (4TMS)]	54	-0,307	-0,491	14,656	0,508	90	51	93	48	67	36 original
3774	31 [622; Parabanic acid (21 40 [860; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0,311	-0,560	40,186	0,530	91	50	105	36	134	27 original
3850	31 [622; Parabanic acid (21 116 [882; Pseudouridine (5TMS)]	30	-0,324	-0,351	9,427	0,338	92	49	74	67	15	134 original
3849	31 [622; Parabanic acid (21 115 Glucose-6-phosphate	62	-0,326	-0,492	30,832	0,443	93	48	94	47	118	82 original
3808	31 [622; Parabanic acid (21 74 [912; Tetradecanoic acid (1TMS)]	64	-0,328	-0,428	13,809	0,447	94	47	85	56	64	80 original
3812	31 [622; Parabanic acid (21 78 Mannose	62	-0,328	-0,488	13,638	0,474	95	46	91	50	61	81 original
3846	31 [622; Parabanic acid (21 112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	-0,330	-0,533	9,838	0,462	96	45	100	41	21	69 original
3834	31 [622; Parabanic acid (21 100 [657; Mannitol (6TMS)]	64	-0,337	-0,535	14,263	0,468	97	44	101	40	65	63 original



3851	31 [622; Parabanic acid (21 117 [724; Glycerol (3TMS)]	56 -0.339	-0.525	12.943	0.490	98	43	98	43	51	47 original
12200	31 [622; Parabanic acid (21 18 [590; 1-Acetyl-2-thiohydantoin]	64 -0.339	-0.446	12.921	0.407	99	42	87	54	50	105 duplicate
3856	31 [622; Parabanic acid (21 122 [644; Erythritol (4TMS)]	52 -0.341	-0.582	14.578	0.485	100	41	106	35	66	50 original
3859	31 [622; Parabanic acid (21 125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64 -0.353	-0.493	38.272	0.434	101	40	95	46	131	91 original
13375	31 [622; Parabanic acid (21 28 Malic acid	64 -0.362	-0.688	14.898	0.533	102	39	121	20	69	22 duplicate
11447	31 [622; Parabanic acid (21 12 Glyceric acid	62 -0.365	-0.676	8.678	0.536	103	38	116	25	11	16 duplicate
3840	31 [622; Parabanic acid (21 106 [733; Threitol (4TMS)]	62 -0.369	-0.551	16.990	0.534	104	37	104	37	79	20 original
3862	31 [622; Parabanic acid (21 128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45 -0.374	-0.518	14.752	0.402	105	36	96	45	68	109 original
3825	31 [622; Parabanic acid (21 91 [766; beta-D-Methylglucopyranoside (4TMS)]	64 -0.382	-0.618	23.063	0.433	106	35	107	34	100	95 original
3772	31 [622; Parabanic acid (21 38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	64 -0.383	-0.728	13.710	0.540	107	34	130	11	62	12 original
3866	31 [622; Parabanic acid (21 132 [895; Isomaltose methoxyamine (8TMS)]	42 -0.384	-0.739	15.558	0.517	108	33	136	5	72	34 original
11702	31 [622; Parabanic acid (21 14 Fumaric acid	64 -0.392	-0.697	8.249	0.548	109	32	123	18	9	7 duplicate
13148	31 [622; Parabanic acid (21 26 Citramalic acid	64 -0.394	-0.647	21.823	0.480	110	30	111	30	97	54 duplicate
3835	31 [622; Parabanic acid (21 101 [832; Dopamine (4TMS)]	64 -0.394	-0.650	16.907	0.422	111	31	112	29	78	101 original
13487	31 [622; Parabanic acid (21 29 Erythritol	64 -0.399	-0.722	9.965	0.537	112	29	129	12	22	14 duplicate
3821	31 [622; Parabanic acid (21 87 [945; beta-D-Glucopyranose (5TMS)]	62 -0.399	-0.546	41.254	0.425	113	28	103	38	136	99 original
11318	31 [622; Parabanic acid (21 11 Succinic acid	64 -0.404	-0.638	13.298	0.508	114	27	109	32	56	35 duplicate
3854	31 [622; Parabanic acid (21 120 [945; Uridine (3TMS)]	54 -0.405	-0.436	17.707	0.541	115	26	86	55	83	9 original
3804	31 [622; Parabanic acid (21 70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57 -0.411	-0.390	23.628	0.383	116	25	80	61	104	116 original
9973	31 [622; Parabanic acid (21 1 [938; Sulfuric acid (2TMS)]	36 -0.432	-0.635	12.099	0.473	117	24	108	33	43	62 duplicate
12077	31 [622; Parabanic acid (21 17 [700; 2-methyl-1,2-propanediol (2TMS)]	64 -0.433	-0.659	24.175	0.464	118	23	114	27	106	67 duplicate
3820	31 [622; Parabanic acid (21 86 [793; D-Galactono-1,4-lactone (4TMS)]	61 -0.433	-0.644	28.701	0.519	119	22	110	31	115	31 original
12917	31 [622; Parabanic acid (21 24 [725; 2-Ketocacetic acid (2TMS)]	64 -0.443	-0.738	38.543	0.525	120	21	135	6	133	28 duplicate
11953	31 [622; Parabanic acid (21 16 [644; 2-Methyl-1,3-butanediol (2TMS)]	64 -0.449	-0.740	24.264	0.524	121	20	137	4	107	29 duplicate
3773	31 [622; Parabanic acid (21 39 [829; 1-Phenylethanol (1TMS)]	63 -0.452	-0.734	23.558	0.541	122	19	133	8	102	11 original
3831	31 [622; Parabanic acid (21 97 [756; beta-D-Methylglucopyranoside (4TMS)]	52 -0.454	-0.688	28.044	0.433	123	18	113	28	114	94 original
12553	31 [622; Parabanic acid (21 21 [678; N,N-DH(2-Hydroxyethyl)-methanamine (2TMS)]	64 -0.458	-0.686	22.519	0.503	124	17	118	23	98	39 duplicate
3822	31 [622; Parabanic acid (21 88 Gluconic acid	64 -0.460	-0.712	18.925	0.483	125	16	128	15	88	51 original
3790	31 [622; Parabanic acid (21 56 [828; Orotic acid (3TMS)]	64 -0.462	-0.709	15.712	0.535	126	15	125	16	73	18 original
3837	31 [622; Parabanic acid (21 103 [648; Ethylamine (2TMS)]	63 -0.466	-0.699	20.962	0.474	127	14	124	17	96	60 original
12682	31 [622; Parabanic acid (21 22 [690; N,N-DH(2-Hydroxyethyl)-methanamine (2TMS)]	52 -0.468	-0.754	11.182	0.531	128	13	138	3	34	26 duplicate
3833	31 [622; Parabanic acid (21 99 [682; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41 -0.468	-0.737	11.479	0.465	129	12	134	7	38	65 original
3780	31 [622; Parabanic acid (21 46 Arabinose	64 -0.472	-0.694	24.781	0.541	130	11	122	19	109	10 original
3826	31 [622; Parabanic acid (21 92 [680; Glycerol-2-phosphate (4TMS)]	54 -0.480	-0.474	13.522	0.376	131	10	89	52	60	123 original
3868	31 [622; Parabanic acid (21 134 Isomaltose	64 -0.487	-0.730	32.392	0.537	132	9	132	9	121	15 original
3789	31 [622; Parabanic acid (21 65 [646; 3-Deoxyglucitol (5TMS)]	63 -0.492	-0.714	18.743	0.564	133	8	127	14	86	2 original
11575	31 [622; Parabanic acid (21 13 Uracil	64 -0.501	-0.758	23.188	0.517	134	7	139	2	101	33 duplicate
3788	31 [622; Parabanic acid (21 54 [NA]	55 -0.502	-0.879	13.191	0.478	135	6	117	24	54	56 original
3791	31 [622; Parabanic acid (21 [757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55 -0.514	-0.688	20.820	0.533	136	5	120	21	95	21 original
3796	31 [622; Parabanic acid (21 62 [812; D-Xylofuranose (4TMS)]	64 -0.516	-0.686	19.949	0.540	137	4	119	22	91	13 original
3853	31 [622; Parabanic acid (21 Glic	59 -0.520	-0.729	17.769	0.488	138	3	131	10	84	48 original
3784	31 [622; Parabanic acid (21 50 [746; Ribonic acid-1,4-lactone (3TMS)]	61 -0.523	-0.763	13.716	0.505	139	2	140	1	63	37 original
3839	31 [622; Parabanic acid (21 105 [705; 2-Ketogluconic acid (5TMS)]	48 -0.546	-0.716	18.886	0.418	140	1	128	13	87	102 original
13599	32 [728; N,N-Dimethyllysine 30 [815; Ethyl-3(2H)-thiophenone]	63 0.714	0.902	33.674	0.568	1	140	5	138	119	48 duplicate
3865	32 [728; N,N-Dimethyllysine 42 Glutamic acid	60 0.698	0.963	29.434	0.643	2	139	1	140	110	9 original
3924	32 [728; N,N-Dimethyllysine 81 Tyrosine	63 0.683	0.867	38.009	0.610	3	138	10	131	128	25 original
3912	32 [728; N,N-Dimethyllysine 69 Arginine	60 0.678	0.934	22.037	0.688	4	137	2	139	84	2 original
3902	32 [728; N,N-Dimethyllysine 59 Ornithine; Arginine	63 0.677	0.873	46.485	0.572	5	136	8	133	138	44 original

3920	32 [728; N,N-Dimethyllysine]	62	0.667	0.917	32,106	0.587	6	135	3	138	117	36 original
10113	32 [728; N,N-Dimethyllysine]	62	0.660	0.852	19,023	0.542	7	134	13	128	60	56 duplicate
3876	32 [728; N,N-Dimethyllysine]	63	0.657	0.873	11,625	0.598	8	133	7	134	9	32 original
11058	32 [728; N,N-Dimethyllysine]	62	0.655	0.869	28,788	0.558	9	132	9	132	107	51 duplicate
3877	32 [728; N,N-Dimethyllysine]	63	0.624	0.810	37,949	0.593	10	131	17	124	128	33 original
11189	32 [728; N,N-Dimethyllysine]	63	0.823	0.834	23,432	0.598	11	130	15	126	88	31 duplicate
13709	32 [728; N,N-Dimethyllysine]	63	0.609	0.779	9,764	0.538	12	129	22	119	6	60 duplicate
3925	32 [728; N,N-Dimethyllysine]	39	0.584	0.832	13,513	0.668	13	128	16	125	19	4 original
10251	32 [728; N,N-Dimethyllysine]	62	0.582	0.770	9,099	0.496	14	127	24	117	4	82 duplicate
3894	32 [728; N,N-Dimethyllysine]	44	0.581	0.862	16,044	0.634	15	126	12	129	37	11 original
10926	32 [728; N,N-Dimethyllysine]	55	0.580	0.737	17,774	0.484	16	125	25	116	53	92 duplicate
3880	32 [728; N,N-Dimethyllysine]	63	0.560	0.845	29,391	0.544	17	124	14	127	109	55 original
3911	32 [728; N,N-Dimethyllysine]	19	0.544	0.887	10,890	0.587	18	123	6	135	8	35 original
3909	32 [728; N,N-Dimethyllysine]	63	0.528	0.776	11,757	0.540	19	122	23	118	10	58 original
10524	32 [728; N,N-Dimethyllysine]	45	0.523	0.906	4,860	0.721	20	121	4	137	1	1 duplicate
10783	32 [728; N,N-Dimethyllysine]	63	0.510	0.799	38,590	0.525	21	120	19	122	125	67 duplicate
13263	32 [728; N,N-Dimethyllysine]	53	0.502	0.862	10,086	0.657	22	119	11	130	7	5 duplicate
12801	32 [728; N,N-Dimethyllysine]	63	0.490	0.801	12,255	0.652	23	118	18	123	13	6 duplicate
3891	32 [728; N,N-Dimethyllysine]	63	0.482	0.670	13,112	0.564	24	117	30	111	17	49 original
3898	32 [728; N,N-Dimethyllysine]	60	0.476	0.574	16,590	0.509	25	116	35	106	42	77 original
3918	32 [728; N,N-Dimethyllysine]	63	0.475	0.782	45,498	0.496	26	115	21	120	137	83 original
3941	32 [728; N,N-Dimethyllysine]	48	0.459	0.730	12,691	0.630	27	114	26	115	15	12 original
3979	32 [728; N,N-Dimethyllysine]	17	0.441	0.599	7,288	0.298	28	113	33	108	2	139 original
3803	32 [728; N,N-Dimethyllysine]	63	0.432	0.683	27,995	0.495	29	112	28	113	104	84 original
3932	32 [728; N,N-Dimethyllysine]	35	0.429	0.592	12,098	0.582	30	111	34	107	11	41 original
3910	32 [728; N,N-Dimethyllysine]	63	0.428	0.678	30,829	0.442	31	110	29	112	115	113 original
3901	32 [728; N,N-Dimethyllysine]	63	0.419	0.690	21,513	0.472	32	109	27	114	81	100 original
3898	32 [728; N,N-Dimethyllysine]	43	0.398	0.519	19,854	0.556	33	108	37	104	63	52 original
3974	32 [728; N,N-Dimethyllysine]	54	0.367	0.424	13,694	0.552	34	107	42	99	20	53 original
13034	32 [728; N,N-Dimethyllysine]	47	0.343	0.792	8,592	0.583	35	106	20	121	3	39 duplicate
3938	32 [728; N,N-Dimethyllysine]	50	0.337	0.462	16,114	0.462	36	105	39	102	38	105 original
3886	32 [728; N,N-Dimethyllysine]	59	0.316	0.399	13,773	0.458	37	104	45	96	21	107 original
3951	32 [728; N,N-Dimethyllysine]	63	0.315	0.467	12,467	0.392	38	103	38	103	14	125 original
3879	32 [728; N,N-Dimethyllysine]	63	0.312	0.646	34,363	0.520	39	102	31	110	122	71 original
3804	32 [728; N,N-Dimethyllysine]	63	0.304	0.327	14,578	0.414	40	101	49	92	28	120 original
3892	32 [728; N,N-Dimethyllysine]	63	0.295	0.387	15,748	0.455	41	100	46	95	33	109 original
3973	32 [728; N,N-Dimethyllysine]	62	0.243	0.408	36,805	0.371	42	99	43	98	128	130 original
10388	32 [728; N,N-Dimethyllysine]	51	0.208	0.571	35,373	0.448	43	98	36	105	123	111 duplicate
12444	20 [619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	31	0.187	0.629	13,922	0.668	44	97	32	109	22	3 duplicate
3895	52 [NA]	45	0.182	0.365	14,870	0.592	45	96	48	93	29	34 original
3914	32 [728; N,N-Dimethyllysine]	63	0.175	0.402	20,321	0.477	46	95	44	97	71	97 original
3867	32 [728; N,N-Dimethyllysine]	58	0.164	0.371	18,319	0.394	47	94	47	94	57	124 original
11828	32 [728; N,N-Dimethyllysine]	63	0.104	0.026	26,395	0.586	48	93	57	84	100	37 duplicate
3906	32 [728; N,N-Dimethyllysine]	51	0.089	0.447	14,427	0.542	49	92	40	101	24	57 original
3907	32 [728; N,N-Dimethyllysine]	62	0.066	0.049	14,534	0.334	50	91	55	86	27	136 original
3892	32 [728; N,N-Dimethyllysine]	37	0.054	0.168	13,149	0.238	51	90	53	88	18	140 original
3862	32 [728; N,N-Dimethyllysine]	63	0.036	0.015	17,024	0.387	52	89	58	83	46	127 original

3950	32 [729; N,N-Dimethyllysini	107	9-(Z)-Octadecenoic acid	63	0.031	0.158	22.623	0.337	53	88	54	87	86	134	original
3980	32 [728; N,N-Dimethyllysini	137	Ergosterol	63	0.016	0.223	21.170	0.397	54	87	50	91	78	122	original
3915	32 [728; N,N-Dimethyllysini	132	D-Xylopyranose (4TMS)]	63	0.006	0.032	15.329	0.356	55	88	56	85	31	132	original
3926	32 [728; N,N-Dimethyllysini	83	Sorbitol	57	0.005	0.440	24.965	0.498	56	85	41	100	93	81	original
3922	32 [729; N,N-Dimethyllysini	79	Glucose	63	0.005	-0.225	42.556	0.491	57	84	69	72	135	89	original
3954	32 [729; N,N-Dimethyllysini	111	[583; Erythritol (4TMS)]	41	-0.002	-0.033	14.520	0.303	58	83	59	82	25	138	original
3981	32 [729; N,N-Dimethyllysini	138	[674; Ergosterol (1TMS)]	45	-0.006	-0.169	12.791	0.417	59	82	52	89	16	118	original
3961	32 [728; N,N-Dimethyllysini	118	[928; Glucopyranose-6-phosphate (6TMS)]	57	-0.008	-0.062	15.834	0.350	60	81	60	81	35	133	original
3976	32 [729; N,N-Dimethyllysini	133	[855; Squalene]	63	-0.065	0.178	15.826	0.447	61	80	51	90	34	112	original
3966	32 [728; N,N-Dimethyllysini	123	[945; Galactofuranose-6-phosphate (7TMS)]	63	-0.078	-0.085	20.008	0.513	62	79	62	79	66	75	original
3933	32 [728; N,N-Dimethyllysini	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	63	-0.079	-0.142	17.149	0.336	63	78	64	77	48	135	original
3937	32 [728; N,N-Dimethyllysini	94	Hexadecenoic acid	63	-0.099	-0.079	29.724	0.467	64	77	61	80	112	102	original
3986	32 [728; N,N-Dimethyllysini	53	Glycerol-2-phosphate	63	-0.104	-0.169	14.187	0.379	65	76	67	74	23	129	original
3984	32 [729; N,N-Dimethyllysini	141	Lanosta-8,24-dien-3-beta-ol	60	-0.110	-0.116	15.227	0.451	66	75	63	78	30	110	original
3939	32 [728; N,N-Dimethyllysini	96	myo-inositol	49	-0.114	-0.153	16.832	0.312	67	74	66	75	44	137	original
3952	32 [729; N,N-Dimethyllysini	109	Octadecenoic acid	63	-0.129	-0.148	30.824	0.460	68	73	65	76	114	106	original
3884	32 [729; N,N-Dimethyllysini	41	[639; Proline (2TMS)]	63	-0.150	-0.178	22.782	0.484	69	72	68	73	87	93	original
3983	32 [728; N,N-Dimethyllysini	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	48	-0.177	-0.243	14.533	0.456	70	71	70	71	26	108	original
3957	32 [729; N,N-Dimethyllysini	114	Fructose-6-phosphate	52	-0.187	-0.395	16.329	0.478	71	70	77	64	40	95	original
3947	32 [729; N,N-Dimethyllysini	104	[795; Erythritol (4TMS)]	62	-0.190	-0.262	17.307	0.487	72	69	71	70	50	91	original
3970	32 [729; N,N-Dimethyllysini	127	[777; Fructose-6-phosphate methoxamine (6TMS)]	38	-0.198	-0.482	16.996	0.380	73	68	85	56	45	128	original
3956	32 [728; N,N-Dimethyllysini	113	Galactose-6-phosphate	61	-0.204	-0.409	17.719	0.468	74	67	80	61	52	101	original
3969	32 [728; N,N-Dimethyllysini	126	[559; Erythritol (4TMS)]	44	-0.209	-0.305	16.502	0.527	75	66	72	69	41	65	original
12323	32 [728; N,N-Dimethyllysini	19	Alanine (BP) (3TMS)	63	-0.216	-0.318	22.028	0.501	76	64	73	68	82	79	duplicate
3890	32 [729; N,N-Dimethyllysini	47	[NA]	63	-0.216	-0.353	20.594	0.492	77	65	75	66	73	87	original
3975	32 [729; N,N-Dimethyllysini	132	[895; Isomaltose methoxamine (8TMS)]	41	-0.229	-0.346	12.223	0.367	78	63	113	28	77	104	original
3959	32 [728; N,N-Dimethyllysini	116	[882; Pseudouridine (5TMS)]	30	-0.241	-0.346	12.223	0.367	79	62	74	67	12	131	original
3936	32 [728; N,N-Dimethyllysini	93	[607; Putrescine (4TMS)]	59	-0.252	-0.479	19.016	0.429	80	61	84	57	59	116	original
3927	32 [728; N,N-Dimethyllysini	84	Mannitol	61	-0.259	-0.691	40.670	0.515	81	60	107	34	131	74	original
12201	32 [729; N,N-Dimethyllysini	18	[590; 1-Acetyl-2-thiohydantoin]	63	-0.260	-0.398	18.287	0.466	82	59	78	63	56	103	duplicate
3978	32 [728; N,N-Dimethyllysini	135	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	63	-0.275	-0.427	21.331	0.494	83	58	82	59	79	86	original
3923	32 [728; N,N-Dimethyllysini	80	[772; D-Glucose (5TMS)]	61	-0.282	-0.454	39.246	0.420	84	57	83	58	130	117	original
3955	32 [728; N,N-Dimethyllysini	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	62	-0.301	-0.496	15.933	0.520	85	56	87	54	36	72	original
3878	32 [728; N,N-Dimethyllysini	35	Pyrogulamic acid	63	-0.306	-0.563	48.854	0.508	86	55	95	46	139	78	original
10659	32 [729; N,N-Dimethyllysini	6	Glycerol	63	-0.315	-0.492	49.103	0.406	87	54	86	55	140	121	duplicate
3945	32 [728; N,N-Dimethyllysini	102	[904; Galactose methoxamine (5TMS)]	63	-0.341	-0.517	15.655	0.517	88	53	88	53	32	73	original
3963	32 [729; N,N-Dimethyllysini	120	[945; Uridine (3TMS)]	53	-0.358	-0.416	22.521	0.600	89	52	81	60	85	28	original
13149	32 [729; N,N-Dimethyllysini	26	Citramalic acid	63	-0.372	-0.639	25.181	0.522	90	51	102	39	96	70	duplicate
3971	32 [728; N,N-Dimethyllysini	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	44	-0.381	-0.620	20.894	0.392	91	50	100	41	75	126	original
3887	32 [728; N,N-Dimethyllysini	44	[910; 2-Ketogluconic acid methoxamine (4TMS)]	49	-0.381	-0.548	22.028	0.475	92	49	91	50	83	98	original
3958	32 [728; N,N-Dimethyllysini	115	Glucose-6-phosphate	61	-0.384	-0.573	34.147	0.623	93	48	86	45	121	68	original
3917	32 [728; N,N-Dimethyllysini	74	[912; Tetradecanoic acid (1TMS)]	63	-0.386	-0.407	19.951	0.567	94	47	79	62	65	47	original
3934	32 [728; N,N-Dimethyllysini	91	[766; beta-D-Methylglucopyranoside (4TMS)]	63	-0.393	-0.708	29.591	0.511	95	46	110	31	111	76	original
3943	32 [728; N,N-Dimethyllysini	100	[857; Mannitol (6TMS)]	63	-0.396	-0.644	19.728	0.535	96	45	104	37	62	61	original
3928	32 [728; N,N-Dimethyllysini	85	[529; Methylcitric acid (4TMS)]	48	-0.404	-0.610	9.463	0.613	97	44	98	43	5	21	original
3916	32 [728; N,N-Dimethyllysini	73	[708; Glucose methoxamine (5TMS)]	57	-0.409	-0.519	18.668	0.498	98	43	89	52	58	80	original
3953	32 [728; N,N-Dimethyllysini	110	[715; Erythritol (4TMS)]	53	-0.414	-0.593	21.433	0.613	99	42	97	44	80	23	original
3968	32 [728; N,N-Dimethyllysini	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	63	-0.414	-0.551	41.009	0.490	100	41	92	49	132	90	original
3964	32 [728; N,N-Dimethyllysini	121	[657; Erythritol (4TMS)]	54	-0.419	-0.529	17.518	0.482	101	40	90	51	51	94	original
3930	32 [728; N,N-Dimethyllysini	87	[945; beta-D-Glucopyranose (5TMS)]	61	-0.423	-0.557	43.470	0.441	102	39	93	48	136	114	original

3944	32 [729; N,N-Dimethyllysine]	101	[832; Dopamine (4TMS)]	63	-0.423	-0.729	23.841	0.494	103	38	112	29	91	85 original
3955	32 [729; N,N-Dimethyllysine]	122	[644; Erythritol (4TMS)]	51	-0.424	-0.657	20.893	0.547	104	37	105	38	74	54 original
9974	32 [729; N,N-Dimethyllysine]	1	[938; Sulfuric acid (2TMS)]	35	-0.429	-0.705	17.982	0.436	105	36	109	32	55	115 duplicate
12564	32 [729; N,N-Dimethyllysine]	21	[878; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	63	-0.430	-0.718	26.332	0.564	106	35	111	30	99	60 duplicate
3919	32 [729; N,N-Dimethyllysine]	76	Fructose	63	-0.436	-0.631	35.782	0.534	107	34	101	40	124	62 original
3913	32 [729; N,N-Dimethyllysine]	107	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	-0.442	-0.385	26.274	0.394	108	33	76	65	98	123 original
3960	32 [729; N,N-Dimethyllysine]	117	[724; Glycerol (3TMS)]	55	-0.444	-0.612	19.885	0.530	109	32	89	42	84	83 original
13376	32 [729; N,N-Dimethyllysine]	28	Malic acid	63	-0.446	-0.772	20.266	0.616	110	31	118	23	69	18 duplicate
3883	32 [729; N,N-Dimethyllysine]	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	63	-0.455	-0.695	41.925	0.598	111	30	108	33	134	30 original
3949	32 [729; N,N-Dimethyllysine]	106	[733; Threitol (4TMS)]	61	-0.459	-0.663	23.451	0.611	112	29	106	35	89	24 original
11448	32 [729; N,N-Dimethyllysine]	12	Glyceric acid	62	-0.480	-0.810	16.733	0.578	113	28	124	17	43	42 duplicate
3921	32 [729; N,N-Dimethyllysine]	78	Mannose	61	-0.480	-0.642	21.019	0.525	114	27	103	38	76	66 original
11319	32 [729; N,N-Dimethyllysine]	11	Succinic acid	63	-0.485	-0.753	19.244	0.566	115	26	116	25	61	48 duplicate
3940	32 [729; N,N-Dimethyllysine]	97	[756; beta-D-Methylglucopyranoside (4TMS)]	51	-0.487	-0.743	33.686	0.478	116	25	114	27	120	96 original
12683	32 [729; N,N-Dimethyllysine]	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	51	-0.492	-0.800	17.256	0.582	117	24	121	20	49	40 duplicate
11703	32 [729; N,N-Dimethyllysine]	14	Fumaric acid	63	-0.493	-0.800	16.309	0.621	118	23	122	19	39	14 duplicate
3946	32 [729; N,N-Dimethyllysine]	103	[648; Ethylamine (2TMS)]	62	-0.512	-0.789	27.704	0.523	119	22	120	21	103	69 original
3881	32 [729; N,N-Dimethyllysine]	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	63	-0.523	-0.847	20.020	0.617	120	21	133	8	67	17 original
3905	32 [729; N,N-Dimethyllysine]	62	[812; D-Xylofuranose (4TMS)]	63	-0.544	-0.743	24.157	0.584	121	20	115	26	92	38 original
13488	32 [729; N,N-Dimethyllysine]	29	Erythritol	63	-0.552	-0.869	17.050	0.645	122	19	135	6	47	8 duplicate
3935	32 [729; N,N-Dimethyllysine]	92	[680; Glycerol-2-phosphate (4TMS)]	53	-0.553	-0.563	20.113	0.415	123	18	94	47	68	119 original
12078	32 [729; N,N-Dimethyllysine]	17	[700; 2-methyl-1,2-propanediol (2TMS)]	63	-0.564	-0.816	28.879	0.571	124	17	126	15	108	45 duplicate
3931	32 [729; N,N-Dimethyllysine]	88	Gluconic acid	63	-0.582	-0.816	25.047	0.604	125	16	125	16	95	27 original
3897	32 [729; N,N-Dimethyllysine]	54	[NA]	54	-0.584	-0.781	20.550	0.492	126	15	119	22	72	88 original
3899	32 [729; N,N-Dimethyllysine]	56	[829; Orotic acid (3TMS)]	63	-0.585	-0.821	23.462	0.608	127	14	128	13	90	26 original
3948	32 [729; N,N-Dimethyllysine]	105	[705; 2-Ketogluconic acid (5TMS)]	47	-0.593	-0.845	25.812	0.474	128	13	132	9	97	99 original
3942	32 [729; N,N-Dimethyllysine]	86	[662; Ribose-5-phosphate methoxamine (BP) (5TMS)]	40	-0.603	-0.850	17.799	0.529	129	12	134	7	54	64 original
11854	32 [729; N,N-Dimethyllysine]	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	63	-0.609	-0.894	28.716	0.649	130	11	136	3	106	7 duplicate
12918	32 [729; N,N-Dimethyllysine]	24	[725; 2-Ketooctanoic acid (2TMS)]	63	-0.610	-0.878	41.493	0.626	131	10	136	5	133	13 duplicate
3977	32 [729; N,N-Dimethyllysine]	134	Isomaltose	63	-0.611	-0.844	37.125	0.618	132	9	131	10	127	15 original
3972	32 [729; N,N-Dimethyllysine]	129	[840; Maltose methoxamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	58	-0.631	-0.840	24.980	0.538	133	8	129	12	94	59 original
3889	32 [729; N,N-Dimethyllysine]	46	Arabinose	63	-0.641	-0.819	31.039	0.618	134	7	127	14	116	16 original
11576	32 [729; N,N-Dimethyllysine]	13	Uracil	63	-0.643	-0.895	28.494	0.634	135	6	139	2	105	10 duplicate
3928	32 [729; N,N-Dimethyllysine]	86	[793; D-Galactono-1,4-lactone (4TMS)]	60	-0.644	-0.771	33.651	0.599	136	5	117	24	118	28 original
3882	32 [729; N,N-Dimethyllysine]	39	[829; 1-Phenylethanol (1TMS)]	62	-0.650	-0.878	29.783	0.614	137	4	137	4	113	19 original
3908	32 [729; N,N-Dimethyllysine]	65	[646; 3-Deoxyglucitol (5TMS)]	62	-0.665	-0.840	26.454	0.613	138	3	130	11	101	22 original
3900	32 [729; N,N-Dimethyllysine]	57	[757; 2-Desoxy-pentose-3-ylose dimethoxamine (2TMS)]	54	-0.677	-0.801	27.532	0.575	139	2	123	18	102	43 original
3893	32 [729; N,N-Dimethyllysine]	50	[746; Ribonic acid-1,4-lactone (3TMS)]	60	-0.689	-0.899	20.311	0.614	140	1	140	1	70	20 original
13600	33 Methionine	30	[815; Ethyl-3(2H)-thiophenone]	64	0.889	0.944	24.271	0.574	1	140	1	140	116	9 duplicate
3985	33 Methionine	34	Aspartic acid	64	0.743	0.918	28.308	0.652	2	139	2	139	127	1 original
10927	33 Methionine	8	Isoleucine	55	0.732	0.534	13.523	0.488	3	138	31	110	39	42 duplicate
11059	33 Methionine	9	Proline	63	0.732	0.718	21.833	0.454	4	137	13	128	105	68 duplicate
4020	33 Methionine	69	Arginine	60	0.725	0.858	14.279	0.577	5	136	5	136	45	8 original
3993	33 Methionine	42	Glutamic acid	60	0.710	0.887	22.369	0.592	6	135	3	138	109	7 original
4010	33 Methionine	59	Ornithine; Arginine	64	0.690	0.810	37.215	0.519	7	134	7	134	138	27 original
10525	33 Methionine	5	Leucine	45	0.673	0.840	9.719	0.641	8	133	6	135	8	2 duplicate
3966	33 Methionine	45	Homocysteine	61	0.662	0.708	22.560	0.483	9	132	15	128	110	44 original
4002	33 Methionine	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	0.658	0.802	22.342	0.604	10	131	8	133	108	5 original
13819	33 Methionine	32	[729; N,N-Dimethyllysine methyl ester]	63	0.657	0.873	11.625	0.598	11	130	4	137	20	6 duplicate

4032	33 Methionine	81 Tyrosine	64 0.654	0.698	29.588	0.467	12	129	17	124	129	54 original
4018	33 Methionine	68 [570; Hypoxanthine (2TMS)]	20 0.653	0.715	15.066	0.528	13	128	14	127	54	21 original
4028	33 Methionine	77 [826; beta-[(5-methyl-2-thienyl)methyleneamino-benzeneacetic acid methyl ester]	62 0.651	0.781	24.125	0.475	14	127	10	131	115	47 original
13710	33 Methionine	31 [622; Parabenic acid (2TMS)]	64 0.645	0.635	11.581	0.519	15	126	23	118	18	29 duplicate
10114	33 Methionine	2 Serine	62 0.626	0.688	13.188	0.469	16	125	19	122	35	52 duplicate
11190	33 Methionine	10 Glycine	64 0.625	0.687	14.774	0.512	17	124	18	123	51	33 duplicate
3988	33 Methionine	37 Phenylalanine	64 0.622	0.725	19.913	0.461	18	123	12	129	96	59 original
4033	33 Methionine	82 Lysine	39 0.595	0.744	10.640	0.561	19	122	11	130	13	12 original
12802	33 Methionine	23 Homoserine	64 0.592	0.679	7.400	0.571	20	121	20	121	2	10 duplicate
10252	33 Methionine	3 Ethanolamine	62 0.549	0.601	11.619	0.444	21	120	26	115	19	70 duplicate
10794	33 Methionine	7 Threonine	64 0.549	0.706	27.103	0.456	22	119	16	125	123	63 duplicate
4006	33 Methionine	55 [612; 4-Aminobutyric acid (2TBS)]	43 0.530	0.464	24.322	0.568	23	118	34	107	117	11 original
3999	33 Methionine	48 Asparagine	64 0.528	0.595	8.963	0.484	24	117	27	114	5	43 original
4049	33 Methionine	98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	48 0.527	0.652	19.091	0.543	25	116	22	119	86	14 original
4040	33 Methionine	89 [775; Dopamine (4TMS)]	35 0.519	0.623	16.115	0.544	26	115	24	117	60	13 original
13264	33 Methionine	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53 0.496	0.790	17.574	0.607	27	114	9	132	71	4 duplicate
4017	33 Methionine	66 Glycine acid-3-phosphate	64 0.496	0.544	9.228	0.440	28	113	30	111	6	72 original
4012	33 Methionine	61 [NA]	64 0.484	0.434	8.561	0.390	29	112	38	103	4	102 original
13035	33 Methionine	25 [708; 2,5-Diaminovalerolactam (2TMS)]	48 0.479	0.658	11.124	0.400	30	111	21	120	16	96 duplicate
4018	33 Methionine	67 Citric acid	64 0.452	0.514	21.350	0.362	31	110	33	108	102	117 original
4046	33 Methionine	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50 0.438	0.446	21.473	0.473	32	109	36	105	104	49 original
4000	33 Methionine	49 [877; Pyrophosphoric acid (4TMS)]	64 0.424	0.445	20.056	0.378	33	108	37	104	97	109 original
4011	33 Methionine	60 Glycine-3-phosphate	64 0.423	0.515	18.709	0.406	34	107	32	109	84	93 original
4082	33 Methionine	131 [626; 5-Methylthiadenosine (3TMS)]	55 0.383	0.370	17.684	0.436	35	106	42	99	73	77 original
4026	33 Methionine	75 Lysine	64 0.365	0.609	36.316	0.404	36	105	25	116	137	71 original
4087	33 Methionine	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17 0.353	0.425	4.017	0.194	37	104	39	102	1	140 original
3994	33 Methionine	43 [548; Leucine (2TBS)]	60 0.339	0.455	7.599	0.461	38	103	35	106	3	58 original
12445		20 [618; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31 0.329	0.582	17.267	0.617	39	102	28	113	67	3 duplicate
4009	33 Methionine	58 [636; 4R-Acetalamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64 0.313	0.551	12.910	0.425	40	101	29	112	33	82 original
4003	33 Methionine	52 [NA]	46 0.306	0.374	18.969	0.447	41	100	41	100	85	88 original
4014	33 Methionine	63 Glutamine	52 0.267	0.415	14.074	0.426	42	99	40	101	43	81 original
4059	33 Methionine	108 Octadecanoic acid	64 0.245	0.339	10.169	0.369	43	98	43	98	10	113 original
4022	33 Methionine	71 [731; Erythrose (3TMS)]	64 0.211	0.256	11.440	0.395	44	97	48	93	17	100 original
3887	33 Methionine	36 [596; N-Acetylglutamic acid (2TMS)]	64 0.197	0.310	25.850	0.420	45	96	46	95	121	85 original
10389	33 Methionine	4 Phosphoric acid	51 0.145	0.312	28.799	0.405	46	95	45	96	128	84 duplicate
4081	33 Methionine	130 Trehalose	63 0.106	0.199	27.561	0.343	47	94	50	91	125	124 original
4075	33 Methionine	124 [734; 1-Monodoleglycerol (2TMS); 1-Monohexadecanoglycerol (1TMS)]	59 0.081	0.202	24.577	0.363	48	93	49	92	118	116 original
11830	33 Methionine	15 Alanine	64 0.080	0.009	17.463	0.474	49	92	56	85	70	48 duplicate
4050	33 Methionine	107 9-(Z)-Octadecanoic acid	64 0.060	0.146	13.491	0.345	50	91	51	90	38	123 original
4015	33 Methionine	64 [789; Tyramine (3TMS)]	63 0.040	0.060	9.916	0.339	51	90	54	87	9	127 original
4070	33 Methionine	119 [931; myo-Inositol-2-phosphate (7TMS)]	64 0.032	0.012	11.073	0.386	52	89	55	86	15	104 original
4034	33 Methionine	83 Sorbitol	58 0.025	0.319	17.432	0.412	53	88	44	97	69	89 original
4090	33 Methionine	139 [700; Ergosta-5,7-dien-3-ol]	38 0.024	0.308	17.920	0.238	54	87	47	94	77	139 original
4088	33 Methionine	137 Ergosterol	64 0.005	0.122	14.014	0.399	55	86	52	89	42	97 original
4082	33 Methionine	111 [583; Erythritol (4TMS)]	42 -0.020	-0.078	19.712	0.351	56	85	61	80	92	122 original
4044	33 Methionine	93 [607; Putrescine (4TMS)]	60 -0.024	-0.141	19.518	0.355	57	84	64	77	90	120 original
4041	33 Methionine	90 [910; 9-(Z)-Hexadecanoic acid (1TMS)]	64 -0.048	-0.077	10.583	0.342	58	83	60	81	12	126 original

4089	33	Methionine	138	[674; Ergosterol (1TMS)]	48	-0.055	0.006	17.184	0.304	59	82	57	84	66	136	original
4030	33	Methionine	79	Glucose	64	-0.058	-0.274	33.403	0.424	60	81	73	68	135	84	original
4023	33	Methionine	72	[919; D-Xylopyranose (4TMS)]	63	-0.065	0.005	12.721	0.338	61	80	58	83	31	128	original
4004	33	Methionine	53	Glycerol-2-phosphate	64	-0.071	-0.082	14.250	0.335	62	79	62	79	44	130	original
4084	33	Methionine	133	[855; Squalene]	64	-0.091	0.062	10.860	0.398	63	78	53	88	14	99	original
4069	33	Methionine	118	[928; Glucopyranose-6-phosphate (6TMS)]	58	-0.108	-0.066	12.917	0.315	64	77	59	82	34	134	original
4092	33	Methionine	141	Lanosta-8,24-dien-3-beta-ol	61	-0.117	-0.203	17.604	0.411	65	76	67	74	72	90	original
4045	33	Methionine	94	Hexadecanoic acid	64	-0.122	-0.189	21.119	0.374	66	75	68	75	101	110	original
4078	33	Methionine	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	39	-0.134	-0.337	10.534	0.247	67	74	74	67	11	137	original
4060	33	Methionine	109	Octadecanoic acid	64	-0.145	-0.263	23.128	0.365	68	73	71	70	113	115	original
4035	33	Methionine	84	Mannitol	62	-0.157	-0.429	31.177	0.408	69	72	83	58	131	91	original
4074	33	Methionine	123	[945; Galactofuranose-6-phosphate (7TMS)]	64	-0.177	-0.166	11.974	0.383	70	71	65	78	23	105	original
4047	33	Methionine	96	myo-Inositol	49	-0.192	-0.140	21.444	0.324	71	70	63	78	103	133	original
4091	33	Methionine	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	49	-0.211	-0.226	18.050	0.366	72	69	69	72	79	114	original
4065	33	Methionine	114	Fructose-6-phosphate	53	-0.218	-0.368	13.840	0.335	73	68	76	65	41	131	original
4067	33	Methionine	116	[882; Pseudouridine (5TMS)]	30	-0.218	-0.273	12.474	0.334	74	67	72	69	30	132	original
4086	33	Methionine	135		64	-0.221	-0.354	12.343	0.440	75	66	75	66	28	73	original
3998	33	Methionine	47	[NA]	64	-0.238	-0.223	15.184	0.392	76	65	68	73	58	101	original
9975	33	Methionine	1	[938; Sulfuric acid (2TMS)]	36	-0.244	-0.404	12.289	0.245	77	64	79	62	27	138	duplicate
4083	33	Methionine	132	[895; Isomaltose methoxyamine (8TMS)]	42	-0.252	-0.600	19.467	0.371	78	63	109	32	88	112	original
4053	33	Methionine	113	Galactose-6-phosphate	62	-0.259	-0.409	14.948	0.373	79	62	80	61	53	111	original
4055	33	Methionine	102	[904; Galactose methoxyamine (5TMS)]	64	-0.280	-0.441	12.057	0.435	80	61	86	55	24	78	original
4036	33	Methionine	104	[795; Erythritol (4TMS)]	63	-0.294	-0.471	13.278	0.445	81	60	92	49	37	69	original
4079	33	Methionine	85	[529; Methylcitric acid (4TMS)]	48	-0.298	-0.465	9.289	0.528	82	59	90	51	7	20	original
4063	33	Methionine	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	-0.303	-0.431	13.543	0.354	83	58	84	57	40	121	original
3992	33	Methionine	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	-0.308	-0.444	19.344	0.470	84	57	87	54	87	51	original
4051	33	Methionine	41	[639; Proline (2TMS)]	64	-0.330	-0.259	14.343	0.437	85	56	70	71	46	75	original
4042	33	Methionine	100	[857; Mannitol (6TMS)]	64	-0.339	-0.543	12.081	0.457	86	55	102	39	25	60	original
4077	33	Methionine	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	-0.346	-0.482	22.946	0.414	87	54	94	47	112	87	original
10660	33	Methionine	126	[559; Erythritol (4TMS)]	45	-0.347	-0.381	12.849	0.383	88	53	78	63	32	108	duplicate
3986	33	Methionine	6	Glycerol	64	-0.349	-0.494	39.767	0.381	89	52	95	46	140	108	duplicate
4025	33	Methionine	35	Pyroglutamic acid	64	-0.364	-0.502	39.437	0.477	90	51	96	45	139	48	original
12324	33	Methionine	74	[912; Tetradecanoic acid (1TMS)]	64	-0.370	-0.451	16.693	0.495	91	50	88	53	62	40	original
12202	33	Methionine	19	Alanine (BP) (3TMS)	64	-0.373	-0.376	14.393	0.413	92	49	77	64	48	88	duplicate
4031	33	Methionine	18	[590; 1-Acetyl-2-thiohydantoin]	64	-0.375	-0.473	11.673	0.434	93	48	93	48	21	79	duplicate
4048	33	Methionine	80	[772; D-Glucose (5TMS)]	62	-0.379	-0.421	30.279	0.381	94	47	81	60	130	107	original
4071	33	Methionine	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	-0.391	-0.511	25.009	0.336	95	46	98	43	120	129	original
4024	33	Methionine	120	[845; Uridine (3TMS)]	54	-0.396	-0.439	14.380	0.468	96	45	85	56	47	53	original
4052	33	Methionine	73	[708; Glucose methoxyamine (5TMS)]	57	-0.400	-0.467	16.914	0.439	97	44	91	50	64	74	original
4086	33	Methionine	101	[832; Dopamine (4TMS)]	64	-0.400	-0.506	16.902	0.398	98	43	97	44	83	98	original
11449	33	Methionine	115	Glucose-6-phosphate	62	-0.412	-0.524	24.750	0.456	99	42	99	42	119	61	original
13377	33	Methionine	12	Glycemic acid	63	-0.417	-0.676	16.067	0.499	100	41	124	17	59	38	duplicate
4050	33	Methionine	28	Malic acid	64	-0.424	-0.670	12.392	0.522	101	40	122	19	29	26	duplicate
3995	33	Methionine	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	-0.441	-0.619	14.767	0.311	102	39	111	30	50	135	original
13150	33	Methionine	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	-0.443	-0.571	16.179	0.356	103	38	103	38	61	119	original
4043	33	Methionine	26	Citramalic acid	64	-0.457	-0.579	15.777	0.464	104	37	104	37	57	57	duplicate
11320	33	Methionine	92	[680; Glycero-2-phosphate (4TMS)]	54	-0.461	-0.455	14.930	0.361	105	36	89	52	52	118	original
4054	33	Methionine	11	Succinic acid	64	-0.461	-0.629	12.148	0.498	106	35	113	28	26	39	duplicate
4005	33	Methionine	103	[648; Ethylamine (2TMS)]	63	-0.461	-0.584	20.608	0.456	107	34	105	38	99	82	original
			54	[NA]	55	-0.464	-0.590	17.831	0.432	108	33	107	34	76	80	original

4076	33 Methionine	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64 -0.468	-0.527	31,939	0.455	109	32	100	41	133	65 original
4086	33 Methionine	105 [705; 2-Ketoglucuronic acid (5TMS)]	48 -0.475	-0.596	18,022	0.342	110	31	108	33	78	125 original
13489	33 Methionine	29 Erythritol	64 -0.482	-0.713	11,959	0.534	111	30	132	9	22	16 duplicate
11704	33 Methionine	14 Fumaric acid	64 -0.483	-0.688	14,563	0.529	112	29	127	14	49	17 duplicate
4007	33 Methionine	56 [829; Orotic acid (3TMS)]	64 -0.486	-0.675	19,543	0.526	113	28	123	18	91	23 original
4072	33 Methionine	121 [657; Erythritol (4TMS)]	55 -0.491	-0.588	18,365	0.420	114	27	106	35	81	86 original
4038	33 Methionine	87 [945; beta-D-Glucopyranose (5TMS)]	62 -0.494	-0.532	34,525	0.406	115	26	101	40	136	82 original
3989	33 Methionine	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	64 -0.502	-0.730	13,261	0.526	116	25	135	6	36	24 original
12079	33 Methionine	17 [700; 2-methyl-1,2-propanediol (2TMS)]	64 -0.504	-0.676	19,829	0.480	117	24	125	16	95	45 duplicate
4027	33 Methionine	76 Fructose	64 -0.505	-0.619	27,003	0.472	118	23	112	29	122	50 original
4008	33 Methionine	757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55 -0.508	-0.650	20,842	0.455	119	22	117	24	100	64 original
4061	33 Methionine	110 [715; Erythritol (4TMS)]	54 -0.509	-0.608	18,580	0.437	120	21	110	31	82	76 original
12684	33 Methionine	22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52 -0.511	-0.661	17,155	0.527	121	20	118	23	65	22 duplicate
3991	33 Methionine	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	64 -0.517	-0.704	32,461	0.517	122	18	130	11	134	30 original
12819	33 Methionine	24 [725; 2-Ketooctanoic acid (2TMS)]	64 -0.517	-0.744	31,903	0.529	123	19	137	4	132	18 duplicate
4068	33 Methionine	117 [724; Glycerol (3TMS)]	56 -0.517	-0.640	15,958	0.424	124	17	114	27	58	83 original
4073	33 Methionine	122 [644; Erythritol (4TMS)]	52 -0.520	-0.643	20,480	0.388	125	16	116	25	98	103 original
11955	33 Methionine	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	64 -0.523	-0.747	19,485	0.529	126	15	138	3	89	19 duplicate
4021	33 Methionine	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57 -0.526	-0.425	18,286	0.401	127	14	82	59	80	95 original
12565	33 Methionine	21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64 -0.530	-0.721	17,313	0.537	128	13	134	7	68	15 duplicate
4039	33 Methionine	88 Gluconic acid	64 -0.534	-0.669	17,703	0.504	129	12	121	20	74	36 original
4085	33 Methionine	134 Isomaltose	64 -0.535	-0.714	28,200	0.514	130	11	133	8	126	31 original
4029	33 Methionine	78 Mannose	62 -0.544	-0.662	18,695	0.468	131	10	119	22	83	55 original
4013	33 Methionine	62 [812; D-Xylofuranose (4TMS)]	64 -0.550	-0.640	15,143	0.465	132	9	115	26	55	56 original
3987	33 Methionine	46 Arabinose	64 -0.552	-0.668	23,778	0.514	133	8	128	13	114	32 original
4037	33 Methionine	86 [793; D-Galactono-1,4-lactone (4TMS)]	61 -0.565	-0.668	27,413	0.523	134	7	120	21	124	25 original
4016	33 Methionine	65 [646; 3-Deoxyglucitol (5TMS)]	63 -0.566	-0.712	22,337	0.509	135	6	131	10	107	34 original
4080	33 Methionine	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59 -0.568	-0.699	19,777	0.451	136	5	129	12	94	67 original
11577	33 Methionine	13 Uracil	64 -0.570	-0.744	19,761	0.519	137	4	136	5	93	28 duplicate
3990	33 Methionine	39 [828; 1-Phenylethanol (1TMS)]	63 -0.571	-0.748	22,044	0.509	138	3	139	2	106	35 original
4057	33 Methionine	106 [733; Threitol (4TMS)]	62 -0.589	-0.682	17,784	0.488	139	2	126	15	75	41 original
4001	33 Methionine	50 [746; Ribonic acid-1,4-lactone (3TMS)]	61 -0.628	-0.763	22,649	0.502	140	1	140	1	111	37 original
13601	34 Aspartic acid	30 [815; Ethyl-3(2H)-thiophenone]	64 -0.795	0.964	5,741	0.600	1	140	1	140	1	4 duplicate
13928	34 Aspartic acid	33 Methionine	64 -0.743	0.918	28,308	0.652	2	139	2	139	65	1 duplicate
4127	34 Aspartic acid	69 Arginine	60 -0.834	0.795	16,154	0.566	3	138	7	134	23	9 original
11060	34 Aspartic acid	9 Proline	63 -0.832	0.704	14,892	0.442	4	137	12	129	20	61 duplicate
13820	34 Aspartic acid	32 [729; N,N-Dimethyllysine methyl ester]	63 -0.824	0.810	37,949	0.593	5	136	4	137	115	6 duplicate
4100	34 Aspartic acid	42 Glutamic acid	60 -0.609	0.809	13,834	0.568	6	135	6	135	15	8 original
4135	34 Aspartic acid	77 [826; beta-[(5-methyl-2-thienyl)methyl]eneamino-benzeneacetic acid methyl ester]	62 -0.602	0.773	10,144	0.462	7	134	8	133	10	50 original
10928	34 Aspartic acid	8 Isoleucine	55 -0.800	0.500	20,650	0.467	8	133	32	109	39	45 duplicate
4117	34 Aspartic acid	59 Ornithine; Arginine	64 -0.890	0.853	9,645	0.515	9	132	3	138	7	20 original
10526	34 Aspartic acid	45 Leucine	45 -0.580	0.810	31,761	0.628	10	131	5	138	84	2 duplicate
4103	34 Aspartic acid	45 Homocysteine	61 -0.574	0.682	49,243	0.521	11	130	15	128	139	16 original
4139	34 Aspartic acid	81 Tyrosine	64 -0.569	0.655	8,265	0.444	12	129	18	123	5	60 original
13711	34 Aspartic acid	31 [622; Parabanic acid (2TMS)]	64 -0.547	0.596	37,621	0.485	13	128	24	117	114	38 duplicate
10115	34 Aspartic acid	2 Serine	62 -0.545	0.644	21,962	0.482	14	127	21	120	44	40 duplicate
11191	34 Aspartic acid	10 Glycine	64 -0.537	0.645	16,373	0.489	15	126	20	121	24	36 duplicate
4095	34 Aspartic acid	37 Phenylalanine	64 -0.536	0.657	11,455	0.440	16	125	17	124	12	65 original

4140	34 Aspartic acid	82 Lysine	39 0.530	0.715	17.869	0.558	17	124	11	130	30	10 original
4126	34 Aspartic acid	68 [570; Hypoxanthine (2TMS)]	20 0.526	0.717	30.539	0.505	18	123	10	131	82	27 original
12803	34 Aspartic acid	23 Homoserine	64 0.524	0.652	28.768	0.517	19	122	19	122	69	19 duplicate
4108	34 Aspartic acid	48 Asparagine	64 0.478	0.577	29.837	0.475	20	121	26	115	75	43 original
10795	34 Aspartic acid	7 Threonine	64 0.478	0.696	6.262	0.445	21	120	13	128	2	57 duplicate
4147	34 Aspartic acid	89 [775; Dopamine (4TMS)]	35 0.476	0.589	33.402	0.537	22	119	25	116	97	11 original
10253	34 Aspartic acid	3 Ethanolamine	62 0.460	0.583	37.242	0.431	23	118	27	114	110	70 duplicate
13265	34 Aspartic acid	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53 0.457	0.752	41.339	0.606	24	117	9	132	126	3 duplicate
4109	34 Aspartic acid	51 [498; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44 0.446	0.694	44.701	0.577	25	116	14	127	132	7 original
4124	34 Aspartic acid	66 Glycine acid-3-phosphate	64 0.443	0.543	33.296	0.392	26	115	28	112	94	92 original
13036	34 Aspartic acid	25 [708; 2,5-Diaminovalerolactam (2TMS)]	48 0.420	0.600	32.154	0.395	27	114	23	118	89	87 duplicate
4156	34 Aspartic acid	98 [697; Ribose-5-phosphate methoxamine (5TMS)]	48 0.408	0.518	42.705	0.518	28	113	31	110	130	17 original
4119	34 Aspartic acid	61 [NA]	64 0.408	0.425	30.434	0.391	29	112	35	108	79	93 original
4113	34 Aspartic acid	55 [612; 4-Aminobutyric acid (2TBS)]	43 0.393	0.437	45.928	0.521	30	111	34	107	136	15 original
4125	34 Aspartic acid	67 Citric acid	64 0.376	0.563	10.858	0.358	31	110	28	113	11	112 original
4107	34 Aspartic acid	49 [877; Pyrophosphoric acid (4TMS)]	64 0.369	0.399	46.033	0.376	32	109	37	104	137	103 original
4189	34 Aspartic acid	131 [626; 5-Methylthiadenosine (3TMS)]	55 0.360	0.358	42.258	0.404	33	108	40	101	129	84 original
4153	34 Aspartic acid	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50 0.358	0.371	45.079	0.471	34	107	39	102	135	44 original
4118	34 Aspartic acid	60 Glyceral-3-phosphate	64 0.344	0.480	13.080	0.381	35	106	33	108	14	101 original
4133	34 Aspartic acid	75 Lysine	64 0.305	0.614	9.733	0.448	36	105	22	119	8	55 original
12446												
4110	34 Aspartic acid	20 [619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	31 0.303	0.538	34.800	0.594	37	104	30	111	103	5 duplicate
4101	34 Aspartic acid	52 [NA]	46 0.295	0.321	40.534	0.442	38	103	43	98	124	62 original
4194	34 Aspartic acid	43 [548; Leucine (2TBS)]	60 0.285	0.413	28.272	0.445	39	102	36	105	64	59 original
		136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17 0.279	0.338	14.641	0.172	40	101	41	100	19	140 original
		58 [636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64 0.270	0.661	19.069	0.431	41	100	16	125	34	69 original
4116	34 Aspartic acid	63 Glutamine	52 0.261	0.387	33.353	0.414	42	99	38	103	96	76 original
4121	34 Aspartic acid	108 Octadecenoic acid	64 0.194	0.225	33.952	0.350	43	98	47	94	99	115 original
4166	34 Aspartic acid	71 [731; Erythrose (3TMS)]	64 0.165	0.323	22.265	0.382	44	97	42	99	45	100 original
4094	34 Aspartic acid	36 [596; N-Acetylglutamic acid (2TMS)]	64 0.143	0.255	9.845	0.397	45	96	46	95	9	86 original
4188	34 Aspartic acid	130 Trehalose	63 0.112	0.184	8.023	0.342	46	95	48	93	4	119 original
10390	34 Aspartic acid	4 Phosphoric acid	51 0.067	0.274	7.693	0.374	47	94	45	96	3	104 duplicate
11831	34 Aspartic acid	15 Alanine	64 0.042	0.023	18.415	0.481	48	93	54	87	31	51 duplicate
4165	34 Aspartic acid	107 9-(Z)-Octadecenoic acid	64 0.033	0.042	20.294	0.331	49	92	52	89	38	125 original
4122	34 Aspartic acid	64 [789; Tyramine (3TMS)]	63 0.012	0.076	31.956	0.331	50	91	51	90	88	126 original
		124 [734; 1-Monooctadecyloxyglycerol (2TMS); 1-Monohexadecyloxyglycerol (1TMS)]	59 0.010	0.087	50.551	0.350	51	90	50	91	140	116 original
4182	34 Aspartic acid	83 Sorbitol	58 0.001	0.294	15.056	0.372	52	89	44	97	22	105 original
4141	34 Aspartic acid	119 [831; myc-Inositol-2-phosphate (7TMS)]	64 -0.011	-0.083	29.734	0.341	53	88	58	83	73	120 original
4177	34 Aspartic acid	53 Glycerol-2-phosphate	64 -0.017	-0.101	39.072	0.339	54	87	60	81	119	121 original
4111	34 Aspartic acid	137 Ergosterol	64 -0.022	0.032	24.372	0.384	55	86	53	88	54	98 original
4195	34 Aspartic acid	93 [607; Putrescine (4TMS)]	60 -0.031	-0.111	43.343	0.325	56	85	61	80	131	129 original
4151	34 Aspartic acid	139 [700; Ergosta-5,7-dien-3-ol]	38 -0.047	0.148	38.508	0.249	57	84	49	92	117	138 original
4197	34 Aspartic acid	79 Glucose	64 -0.059	-0.234	12.851	0.393	58	83	68	73	13	89 original
4137	34 Aspartic acid	72 [919; D-Xylopyranose (4TMS)]	63 -0.059	-0.023	34.949	0.338	59	82	56	85	104	122 original
4130	34 Aspartic acid	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	64 -0.070	-0.134	29.294	0.322	60	81	63	78	71	132 original
4148	34 Aspartic acid	111 [583; Erythritol (4TMS)]	42 -0.071	-0.125	41.735	0.257	61	80	62	79	128	136 original
4169	34 Aspartic acid	127 [777; Fructose-6-phosphate methoxamine (6TMS)]	39 -0.085	-0.251	22.547	0.249	62	79	70	71	48	137 original
4185	34 Aspartic acid	118 [928; Glucopyranose-6-phosphate (6TMS)]	58 -0.101	-0.080	33.299	0.321	63	78	57	84	95	133 original
4176	34 Aspartic acid	138 [674; Ergosterol (1TMS)]	46 -0.103	-0.096	39.333	0.281	64	77	59	82	120	135 original



4152	34 Aspartic acid	94	Hexadecanoic acid	64	-0.107	-0.187	17.398	0.361	65	76	66	75	28	109 original
4191	34 Aspartic acid	133	[855; Squalene]	64	-0.116	-0.020	30.468	0.355	68	76	55	86	80	113 original
4199	34 Aspartic acid	141	Lanosta-8,24-dien-3-beta-ol	61	-0.149	-0.262	41.698	0.392	67	74	71	70	127	91 original
4105	34 Aspartic acid	47	[NA]	64	-0.154	-0.189	32.447	0.386	68	73	67	74	91	97 original
4154	34 Aspartic acid	96	myo-Inositol	49	-0.155	-0.142	44.754	0.311	69	72	65	76	133	134 original
4142	34 Aspartic acid	84	Mannitol	62	-0.157	-0.405	16.896	0.378	70	71	88	53	26	102 original
4167	34 Aspartic acid	109	Ocladecanoic acid	64	-0.160	-0.244	21.377	0.366	71	70	69	72	41	97 original
4181	34 Aspartic acid	123	[945; Galactofuranose-6-phosphate (7TMS)]	64	-0.176	-0.139	24.667	0.380	72	69	64	77	55	94 original
4193	34 Aspartic acid	135		64	-0.212	-0.266	22.425	0.405	73	68	72	69	47	83 original
9976	34 Aspartic acid	1	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	36	-0.222	-0.378	23.869	0.208	74	67	85	56	53	139 duplicate
4171	34 Aspartic acid	113	Galactose-6-phosphate	62	-0.248	-0.352	35.264	0.365	75	66	80	61	106	108 original
4186	34 Aspartic acid	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	-0.248	-0.322	22.743	0.323	76	65	77	64	49	130 original
4184	34 Aspartic acid	126	[559; Erythritol (4TMS)]	45	-0.259	-0.274	28.233	0.348	77	64	75	66	63	118 original
4174	34 Aspartic acid	116	[882; Pseudouridine (5TMS)]	30	-0.260	-0.269	26.333	0.325	78	63	73	68	58	128 original
4198	34 Aspartic acid	140	[892; Ergosta-7,22-dien-3-ol (1TMS)]	49	-0.260	-0.321	40.552	0.337	79	62	76	65	125	123 original
4160	34 Aspartic acid	102	[904; Galactose methoxymine (5TMS)]	64	-0.267	-0.347	34.123	0.413	80	61	79	62	100	78 original
4170	34 Aspartic acid	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (8TMS)]	63	-0.268	-0.362	45.045	0.420	81	60	83	58	134	73 original
4172	34 Aspartic acid	114	Fructose-6-phosphate	53	-0.271	-0.360	33.226	0.331	82	59	81	60	93	124 original
4190	34 Aspartic acid	132	[895; Isomaltose methoxymine (8TMS)]	42	-0.294	-0.563	35.591	0.352	83	58	115	26	108	114 original
4093	34 Aspartic acid	35	Pyroglutamic acid	64	-0.298	-0.411	14.351	0.416	84	57	90	51	17	75 original
4162	34 Aspartic acid	104	[795; Erythritol (4TMS)]	63	-0.301	-0.390	31.928	0.414	85	56	86	55	87	77 original
4138	34 Aspartic acid	80	[772; D-Glucose (5TMS)]	62	-0.307	-0.378	16.909	0.357	86	55	84	57	27	111 original
4158	34 Aspartic acid	100	[857; Mannitol (6TMS)]	64	-0.311	-0.458	27.083	0.436	87	54	95	46	61	68 original
4131	34 Aspartic acid	73	[708; Glucose methoxymine (5TMS)]	57	-0.325	-0.333	35.336	0.441	88	53	78	63	107	63 original
10661	34 Aspartic acid	6	Glycerol	64	-0.326	-0.426	14.313	0.371	89	52	93	48	16	106 duplicate
4149	34 Aspartic acid	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	-0.331	-0.480	34.338	0.393	90	51	102	39	101	90 original
4099	34 Aspartic acid	41	[639; Proline (2TMS)]	64	-0.333	-0.271	22.344	0.412	91	50	74	67	46	79 original
4159	34 Aspartic acid	101	[832; Dopamine (4TMS)]	64	-0.349	-0.476	31.779	0.408	92	49	99	42	85	81 original
4155	34 Aspartic acid	97	[758; beta-D-Methylglucopyranoside (4TMS)]	52	-0.359	-0.497	23.631	0.322	93	48	103	38	51	131 original
12325	34 Aspartic acid	19	Alanine (BP) (3TMS)	64	-0.368	-0.361	25.293	0.394	94	47	82	59	56	88 duplicate
4143	34 Aspartic acid	85	[529; Methylepic acid (4TMS)]	48	-0.376	-0.507	28.916	0.497	95	46	104	37	70	32 original
12203	34 Aspartic acid	18	[590; 1-Acetyl-2-thiohydantoin]	64	-0.378	-0.455	28.536	0.429	96	45	94	47	68	71 duplicate
4157	34 Aspartic acid	99	[662; Ribose-5-phosphate methoxymine (BP) (5TMS)]	41	-0.385	-0.528	30.389	0.326	97	44	107	34	78	127 original
4102	34 Aspartic acid	44	[910; 2-Ketogluconic acid methoxymine (4TMS)]	50	-0.386	-0.469	26.683	0.350	98	43	97	44	60	117 original
4178	34 Aspartic acid	120	[945; Uridine (3TMS)]	54	-0.388	-0.426	21.321	0.453	99	42	92	49	40	54 original
4150	34 Aspartic acid	92	[680; Glycerol-2-phosphate (4TMS)]	54	-0.391	-0.405	30.332	0.358	100	41	89	52	77	110 original
4132	34 Aspartic acid	74	[912; Tetradecanoic acid (1TMS)]	64	-0.395	-0.418	35.256	0.460	101	40	91	50	105	52 original
4173	34 Aspartic acid	115	Glucose-6-phosphate	62	-0.401	-0.472	14.929	0.438	102	39	98	43	21	67 original
4112	34 Aspartic acid	54	[NA]	55	-0.402	-0.509	36.857	0.418	103	38	105	36	109	74 original
4179	34 Aspartic acid	121	[657; Erythritol (4TMS)]	55	-0.409	-0.477	39.436	0.406	104	37	100	41	121	82 original
11450	34 Aspartic acid	12	Glyceric acid	63	-0.413	-0.601	39.463	0.488	105	36	120	21	122	37 duplicate
13378	34 Aspartic acid	28	Malic acid	64	-0.415	-0.611	26.533	0.512	106	35	123	18	59	24 duplicate
4145	34 Aspartic acid	87	[945; beta-D-Glucopyranose (5TMS)]	62	-0.419	-0.478	17.466	0.402	107	34	101	40	29	85 original
13490	34 Aspartic acid	29	Erythritol	64	-0.422	-0.624	32.294	0.512	108	33	126	15	90	25 duplicate
4183	34 Aspartic acid	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	-0.436	-0.468	16.582	0.446	109	32	96	45	25	56 original
4114	34 Aspartic acid	56	[829; Orotic acid (3TMS)]	64	-0.438	-0.589	37.579	0.512	110	31	119	22	112	22 original
4161	34 Aspartic acid	103	[648; Ethylamine (2TMS)]	63	-0.439	-0.550	31.787	0.467	111	30	113	28	86	48 original
4163	34 Aspartic acid	105	[705; 2-Ketogluconic acid (5TMS)]	48	-0.441	-0.546	25.464	0.383	112	28	111	30	57	99 original
4168	34 Aspartic acid	110	[715; Erythritol (4TMS)]	54	-0.445	-0.512	34.759	0.428	113	28	106	35	102	72 original
4096	34 Aspartic acid	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.445	-0.649	29.347	0.512	114	27	134	7	72	23 original

11321	34 Aspartic acid	11 Succinic acid	64 -0.446	-0.564	28.545	0.502	115	26	116	25	67	28 Duplicate
4134	34 Aspartic acid	76 Fructose	64 -0.450	-0.543	19.284	0.439	116	25	110	31	35	66 original
12080	34 Aspartic acid	17 [700; 2-methyl-1,2-propanediol (2TMS)]	64 -0.457	-0.587	21.408	0.463	117	24	118	23	42	48 Duplicate
4180	34 Aspartic acid	122 [644; Erythritol (4TMS)]	52 -0.462	-0.539	39.540	0.389	118	23	108	33	123	95 original
4136	34 Aspartic acid	78 Mannose	62 -0.466	-0.615	37.442	0.463	119	22	124	17	111	49 original
12920	34 Aspartic acid	24 [725; 2-Ketotetanoic acid (2TMS)]	64 -0.468	-0.658	14.494	0.513	120	21	135	6	18	21 Duplicate
4098	34 Aspartic acid	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	64 -0.474	-0.620	9.476	0.493	121	20	125	16	6	35 original
4192	34 Aspartic acid	134 Isomaltose	64 -0.476	-0.643	23.024	0.501	122	19	130	11	60	29 original
4120	34 Aspartic acid	62 [812; D-Xylofuranose (4TMS)]	64 -0.477	-0.541	21.574	0.457	123	18	109	32	43	53 original
4128	34 Aspartic acid	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57 -0.479	-0.404	18.428	0.387	124	17	87	54	32	96 original
4146	34 Aspartic acid	88 Gluconic acid	64 -0.481	-0.610	28.721	0.476	125	16	122	19	68	42 original
11956	34 Aspartic acid	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	64 -0.484	-0.663	20.245	0.509	126	15	138	5	37	26 Duplicate
12685	34 Aspartic acid	22 [690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	52 -0.488	-0.628	38.617	0.527	127	14	129	12	118	13 Duplicate
13151	34 Aspartic acid	26 Citramalic acid	64 -0.488	-0.555	18.576	0.465	128	13	114	27	33	47 Duplicate
4175	34 Aspartic acid	117 [724; Glycerol (3TMS)]	56 -0.490	-0.550	32.452	0.411	129	12	112	29	92	80 original
11705	34 Aspartic acid	14 Fumaric acid	64 -0.490	-0.648	37.610	0.533	130	11	132	9	113	12 Duplicate
4115	34 Aspartic acid	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55 -0.494	-0.609	29.811	0.445	131	10	121	20	74	58 original
4104	34 Aspartic acid	46 Arabinose	64 -0.495	-0.625	30.275	0.501	132	9	128	13	76	30 original
4144	34 Aspartic acid	86 [793; D-Galactono-1,4-lactone (4TMS)]	61 -0.508	-0.625	30.510	0.518	133	8	127	14	81	18 original
4164	34 Aspartic acid	106 [733; Threitol (4TMS)]	62 -0.513	-0.584	30.710	0.480	134	7	117	24	83	41 original
4187	34 Aspartic acid	129 [840; Malbose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59 -0.520	-0.645	33.924	0.440	135	6	131	10	98	64 original
4097	34 Aspartic acid	39 [829; 1-Phenylethanol (1TMS)]	63 -0.524	-0.672	28.082	0.496	136	5	137	4	62	33 original
4123	34 Aspartic acid	65 [646; 3-Deoxyglucitol (5TMS)]	63 -0.525	-0.648	38.420	0.496	137	4	133	8	116	34 original
12566	34 Aspartic acid	21 [678; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	64 -0.529	-0.694	19.769	0.525	138	3	139	2	36	14 Duplicate
11578	34 Aspartic acid	13 Urcil	64 -0.540	-0.677	23.793	0.500	139	2	138	3	52	31 Duplicate
4108	34 Aspartic acid	50 [746; Ribonic acid-1,4-lactone (3TMS)]	61 -0.584	-0.699	47.024	0.484	140	1	140	1	138	39 original
4279	35 Pyrogulamic acid	115 Glucose-6-phosphate	62 0.760	0.957	17.275	0.632	1	140	2	139	16	17 original
4240	35 Pyrogulamic acid	76 Fructose	64 0.736	0.970	19.287	0.671	2	139	1	140	19	2 original
4270	35 Pyrogulamic acid	106 [733; Threitol (4TMS)]	62 0.682	0.883	36.125	0.656	3	138	12	129	70	7 original
13379	35 Pyrogulamic acid	28 Malic acid	64 0.671	0.830	33.900	0.584	4	137	24	117	63	36 Duplicate
4204	35 Pyrogulamic acid	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	64 0.663	0.808	7.692	0.575	5	1				

12686	35 Pyroglutamic acid	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.582	0.740	45,260	0.542	24	117	44	97	113	60 duplicate
12921	35 Pyroglutamic acid	24	[725; 2-Ketooctanoic acid (2TMS)]	64	0.581	0.860	10,896	0.649	25	116	18	123	7	10 duplicate
4208	35 Pyroglutamic acid	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	0.580	0.789	35,049	0.560	26	115	37	104	67	39 original
11322	35 Pyroglutamic acid	11	Succinic acid	64	0.575	0.835	35,983	0.580	27	114	21	120	69	57 duplicate
4298	35 Pyroglutamic acid	134	Isomaltose	64	0.548	0.890	22,382	0.647	28	112	11	130	27	11 original
11957	35 Pyroglutamic acid	16	[844; 2-Methyl-1,3-butanediol (2TMS)]	64	0.548	0.824	25,014	0.635	29	113	26	115	31	15 duplicate
13481	35 Pyroglutamic acid	29	Erythritol	64	0.547	0.794	40,144	0.566	30	111	35	106	92	52 duplicate
13152	35 Pyroglutamic acid	26	Citramalic acid	64	0.544	0.714	25,878	0.472	31	110	48	93	35	93 duplicate
4210	35 Pyroglutamic acid	46	Arabinose	64	0.541	0.913	32,803	0.655	32	109	6	135	58	8 original
4203	35 Pyroglutamic acid	39	[828; 1-Phenylethanol (1TMS)]	63	0.538	0.828	31,364	0.604	33	108	25	116	52	28 original
4276	35 Pyroglutamic acid	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.531	0.634	53,879	0.516	34	107	57	84	136	72 original
4234	35 Pyroglutamic acid	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	0.530	0.725	22,340	0.525	35	106	46	95	26	68 original
4252	35 Pyroglutamic acid	88	Gluconic acid	64	0.519	0.806	33,974	0.634	36	105	33	108	64	16 original
12081	35 Pyroglutamic acid	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	0.513	0.832	25,859	0.541	37	104	23	118	34	62 duplicate
12567	35 Pyroglutamic acid	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	0.507	0.669	25,896	0.483	38	103	51	90	37	89 duplicate
4287	35 Pyroglutamic acid	123	[945; Galactofuranose-6-phosphate (7TMS)]	64	0.503	0.760	32,308	0.543	39	102	41	100	58	59 original
12326	35 Pyroglutamic acid	19	Alanine (BP) (3TMS)	64	0.501	0.809	31,879	0.546	40	101	31	110	53	58 duplicate
4293	35 Pyroglutamic acid	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	0.494	0.863	39,474	0.643	41	100	17	124	89	12 original
4229	35 Pyroglutamic acid	65	[846; 3-Deoxyglucitol (5TMS)]	63	0.490	0.896	43,247	0.665	42	99	10	131	105	4 original
4299	35 Pyroglutamic acid	135	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	0.488	0.503	30,437	0.454	43	98	65	76	48	101 original
11579	35 Pyroglutamic acid	13	Uracil	64	0.486	0.820	28,009	0.620	44	97	28	113	41	21 duplicate
4284	35 Pyroglutamic acid	120	[845; Uridine (3TMS)]	54	0.474	0.256	29,127	0.508	45	96	74	67	46	78 original
11451	35 Pyroglutamic acid	12	Glyceric acid	63	0.470	0.698	47,529	0.510	46	95	50	91	119	76 duplicate
4238	35 Pyroglutamic acid	74	[912; Tetradecanoic acid (1TMS)]	64	0.468	0.591	42,034	0.470	47	94	59	82	99	94 original
12204	35 Pyroglutamic acid	18	[590; 1-Acetyl-2-thiohydantoin]	64	0.461	0.590	36,225	0.413	48	93	60	81	71	118 duplicate
4268	35 Pyroglutamic acid	104	[795; Erythritol (4TMS)]	63	0.456	0.656	38,918	0.523	49	92	53	88	83	69 original
10662	35 Pyroglutamic acid	6	Glycerol	64	0.449	0.840	2,850	0.571	50	91	20	121	1	48 duplicate
4214	35 Pyroglutamic acid	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	0.446	0.789	55,150	0.566	51	90	40	101	137	51 original
4218	35 Pyroglutamic acid	54	[NA]	55	0.433	0.820	45,014	0.575	52	89	27	114	112	45 original
4221	35 Pyroglutamic acid	57	[757; 2-Deoxy-pentose-3-ylose dimethoxyamine (2TMS)]	55	0.425	0.877	35,051	0.599	53	88	14	127	68	30 original
4249	35 Pyroglutamic acid	85	[529; Methylcitric acid (4TMS)]	48	0.424	0.566	33,765	0.432	54	87	61	80	62	111 original
4267	35 Pyroglutamic acid	103	[648; Ethylamine (2TMS)]	63	0.412	0.639	36,558	0.509	55	88	56	85	74	77 original
4280	35 Pyroglutamic acid	116	[882; Pseudouridine (5TMS)]	30	0.411	0.202	31,053	0.503	56	85	76	65	51	81 original
4247	35 Pyroglutamic acid	83	Sorbitol	58	0.400	-0.053	22,210	0.325	57	84	85	56	24	139 original
4205	35 Pyroglutamic acid	41	[639; Proline (2TMS)]	64	0.399	0.826	29,398	0.499	58	83	56	83	47	83 original
4256	35 Pyroglutamic acid	92	[680; Glycerol-2-phosphate (4TMS)]	54	0.375	0.864	38,523	0.557	59	82	16	125	81	54 original
4292	35 Pyroglutamic acid	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.372	0.751	32,222	0.566	60	81	43	98	55	50 original
4265	35 Pyroglutamic acid	101	[832; Dopamine (4TMS)]	64	0.325	0.542	38,020	0.504	61	80	64	77	78	80 original
4228	35 Pyroglutamic acid	64	[789; Tyramine (3TMS)]	63	0.323	0.557	40,534	0.404	62	79	63	78	94	121 original
4243	35 Pyroglutamic acid	79	Glucose	64	0.320	0.810	8,729	0.578	63	78	30	111	5	41 original
11832	35 Pyroglutamic acid	15	Alanine	64	0.315	0.663	25,005	0.599	64	77	52	89	30	31 duplicate
4260	35 Pyroglutamic acid	96	myo-Inositol	49	0.308	0.211	51,459	0.399	65	76	75	68	134	123 original
4281	35 Pyroglutamic acid	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.301	0.335	33,439	0.641	66	75	72	69	60	13 original
4251	35 Pyroglutamic acid	87	[945; beta-D-Glucopyranose (5TMS)]	62	0.267	0.788	11,746	0.538	67	74	38	103	8	64 original
4275	35 Pyroglutamic acid	111	[583; Erythritol (4TMS)]	42	0.264	0.379	51,211	0.490	68	73	68	73	132	85 original
4297	35 Pyroglutamic acid	133	[855; Squalene]	64	0.251	0.165	38,757	0.360	69	72	78	63	82	134 original
4255	35 Pyroglutamic acid	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	0.244	0.461	38,964	0.463	70	71	66	75	84	95 original
4273	35 Pyroglutamic acid	109	Octadecanoic acid	64	0.223	0.425	25,514	0.487	71	70	67	74	32	87 original

4302	35	Pyroglutamic acid	138	[674; Ergosterol (1TMS)]	46	0.210	0.165	47,244	0.486	72	69	77	64	118	88	original
4244	35	Pyroglutamic acid	80	[772; D-Glucose (5TMS)]	62	0.198	0.715	15,079	0.512	73	68	47	94	13	75	original
4268	35	Pyroglutamic acid	94	Hexadecanoic acid	64	0.171	0.305	22,947	0.473	74	67	73	68	28	92	original
4261	35	Pyroglutamic acid	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	0.164	0.558	27,401	0.516	75	66	62	79	40	71	original
4304	35	Pyroglutamic acid	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	49	0.143	0.024	47,771	0.440	76	65	62	59	120	108	original
4263	35	Pyroglutamic acid	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	0.141	0.700	39,353	0.590	77	64	49	92	86	34	original
4269	35	Pyroglutamic acid	105	[705; 2-Keogluconic acid (5TMS)]	48	0.124	0.354	33,530	0.542	78	63	69	72	61	61	original
4235	35	Pyroglutamic acid	71	[731; Erythrose (3TMS)]	64	0.117	-0.030	30,813	0.395	79	62	84	57	49	127	original
4305	35	Pyroglutamic acid	141	Lanosta-8,24-dien-3-beta-ol	61	0.074	-0.091	49,542	0.427	80	61	86	55	128	113	original
4300	35	Pyroglutamic acid	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.074	0.341	22,268	0.532	81	60	70	71	25	67	original
4282	35	Pyroglutamic acid	118	[928; Glucopyranose-6-phosphate (6TMS)]	58	0.055	0.338	41,989	0.475	82	59	71	70	98	91	original
4301	35	Pyroglutamic acid	137	Ergosterol	64	0.036	-0.168	32,583	0.430	83	58	88	53	57	112	original
4303	35	Pyroglutamic acid	139	[700; Ergosta-5,7-dien-3-ol]	38	0.030	-0.175	46,427	0.447	84	57	90	51	115	104	original
4222	35	Pyroglutamic acid	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	-0.018	-0.089	28,874	0.347	85	56	87	54	45	136	original
4248	35	Pyroglutamic acid	84	Mannitol	62	-0.043	0.145	16,313	0.405	86	55	79	62	14	120	original
10766	35	Pyroglutamic acid	7	Threonine	64	-0.046	-0.241	13,137	0.400	87	54	93	48	11	122	duplicate
4288	35	Pyroglutamic acid	124	[734; 1-Monocleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]	59	-0.057	-0.343	59,343	0.445	88	53	101	40	140	105	original
4211	35	Pyroglutamic acid	47	[NA]	64	-0.061	0.025	40,224	0.396	89	52	81	60	93	125	original
4239	35	Pyroglutamic acid	75	Lysine	64	-0.080	-0.220	8,654	0.395	90	51	92	49	4	128	original
4283	35	Pyroglutamic acid	119	[931; myo-Inositol-2-phosphate (7TMS)]	64	-0.082	-0.365	36,344	0.533	91	50	104	37	79	66	original
4257	35	Pyroglutamic acid	93	[607; Putrescine (4TMS)]	60	-0.092	-0.001	51,855	0.423	92	49	83	58	135	114	original
4294	35	Pyroglutamic acid	130	Trehalose	63	-0.089	-0.190	12,916	0.327	93	48	91	50	10	138	original
10391	35	Pyroglutamic acid	4	Phosphoric acid	51	-0.112	-0.175	7,749	0.297	94	47	89	52	3	140	duplicate
10116	35	Pyroglutamic acid	2	Serine	62	-0.131	-0.328	31,947	0.391	95	46	99	42	54	130	duplicate
4200	35	Pyroglutamic acid	36	[596; N-Acetylglutamic acid (2TMS)]	64	-0.131	-0.315	16,562	0.396	96	45	97	44	15	126	original
4217	35	Pyroglutamic acid	53	Glycerol-2-phosphate	64	-0.138	-0.255	47,842	0.380	97	44	95	46	121	132	original
4254	35	Pyroglutamic acid	90	[910; 9-(Z)-Hexadecanoic acid (1TMS)]	64	-0.146	-0.337	37,829	0.406	98	43	100	41	77	119	original
4271	35	Pyroglutamic acid	107	9-(Z)-Octadecanoic acid	64	-0.152	-0.462	26,738	0.417	99	42	107	34	44	115	original
4230	35	Pyroglutamic acid	66	Glycic acid-3-phosphate	64	-0.156	-0.316	42,492	0.397	100	41	98	43	102	124	original
4231	35	Pyroglutamic acid	67	Citric acid	64	-0.176	-0.488	18,852	0.461	101	40	108	32	18	97	original
4224	35	Pyroglutamic acid	60	Glycerol-3-phosphate	64	-0.189	-0.459	21,935	0.462	102	39	106	35	23	96	original
4201	35	Pyroglutamic acid	37	Phenylalanine	64	-0.214	-0.489	20,152	0.445	103	38	111	30	21	106	original
11061	35	Pyroglutamic acid	9	Proline	63	-0.221	-0.374	25,884	0.392	104	37	103	38	36	129	duplicate
13266	35	Pyroglutamic acid	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	-0.237	-0.585	49,011	0.457	105	36	119	22	126	99	duplicate
9977	35	Pyroglutamic acid	1	[938; Sulfuric acid (2TMS)]	36	-0.241	0.141	34,074	0.579	106	35	80	61	65	40	duplicate
4236	35	Pyroglutamic acid	72	[919; D-Xylopyranose (4TMS)]	63	-0.251	-0.255	43,365	0.356	107	34	94	47	107	135	original
10929	35	Pyroglutamic acid	8	Isoleucine	55	-0.266	-0.311	28,332	0.330	108	33	96	45	43	137	duplicate
13712	35	Pyroglutamic acid	31	[622; Parabanic acid (2TMS)]	64	-0.273	-0.488	47,226	0.433	109	32	110	31	117	109	duplicate
4272	35	Pyroglutamic acid	108	Octadecanoic acid	64	-0.280	-0.505	43,095	0.414	110	31	114	27	104	117	original
14036	35	Pyroglutamic acid	34	Aspartic acid	64	-0.298	-0.411	14,351	0.416	111	30	105	36	12	116	duplicate
13821	35	Pyroglutamic acid	32	[729; N,N-Dimethyllysine methyl ester]	63	-0.306	-0.563	48,854	0.508	112	29	117	24	125	79	duplicate
10254	35	Pyroglutamic acid	3	Ethanolamine	62	-0.353	-0.763	46,685	0.582	113	28	129	12	116	37	duplicate
4207	35	Pyroglutamic acid	43	[546; Leucine (2TBS)]	60	-0.354	-0.359	36,397	0.492	114	27	102	39	72	84	original
4262	35	Pyroglutamic acid	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	64	-0.355	-0.627	50,003	0.433	115	26	121	20	129	110	original
12804	35	Pyroglutamic acid	23	Homoserine	64	-0.357	-0.653	39,381	0.500	116	25	122	19	87	82	duplicate
4225	35	Pyroglutamic acid	61	[NA]	64	-0.358	-0.525	39,619	0.514	117	24	115	26	90	74	original
13929	35	Pyroglutamic acid	33	Methionine	64	-0.364	-0.502	39,437	0.477	118	23	112	29	88	90	duplicate
13602	35	Pyroglutamic acid	30	[815; Ethyl-3(2H)-thiophenone]	64	-0.372	-0.471	19,448	0.370	119	22	108	33	20	133	duplicate
4223	35	Pyroglutamic acid	59	Ornithine; Arginine	64	-0.376	-0.503	9,727	0.442	120	21	113	28	6	107	original

4245	35	Pyroglutamic acid	81	Tyrosine	64	-0.379	-0.748	17.526	0.609	121	20	128	13	17	27	original
4216	35	Pyroglutamic acid	52	[NA]	46	-0.399	-0.841	48.721	0.614	122	19	132	9	124	24	original
4232	35	Pyroglutamic acid	68	[570; Hypoxanthine (2TMS)]	20	-0.400	-0.929	33.310	0.612	123	18	137	4	59	26	original
4241	35	Pyroglutamic acid	77	[826; beta-[[[5-methyl-2-thienyl)methyl]eneamino- benzeneacetic acid methyl ester]	62	-0.403	-0.617	21.819	0.455	124	17	120	21	22	100	original
4209	35	Pyroglutamic acid	45	Homocysteine	61	-0.442	-0.554	57.974	0.395	125	16	116	25	139	131	original
4233	35	Pyroglutamic acid	69	Arginine	60	-0.446	-0.729	26.832	0.571	126	15	127	14	38	47	original
1192	35	Pyroglutamic acid	10	Glycine	64	-0.485	-0.854	27.350	0.630	127	14	133	8	39	18	duplicate
4227	35	Pyroglutamic acid	63	Glutamine	52	-0.498	-0.877	44.058	0.668	128	13	135	6	110	3	original
4206	35	Pyroglutamic acid	42	Glutamic acid	60	-0.498	-0.585	24.411	0.458	129	12	118	23	29	88	original
4215	35	Pyroglutamic acid	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.499	-0.668	49.276	0.453	130	11	124	17	127	102	original
4259	35	Pyroglutamic acid	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	-0.513	-0.785	51.289	0.515	131	10	130	11	133	73	original
4253	35	Pyroglutamic acid	89	[775; Dopamine (4TMS)]	35	-0.523	-0.944	38.990	0.621	132	9	139	2	85	20	original
4212	35	Pyroglutamic acid	48	Asparagine	64	-0.527	-0.862	40.722	0.636	133	8	134	7	96	14	original
10527	35	Pyroglutamic acid	5	Leucine	45	-0.554	-0.655	37.562	0.448	134	7	123	18	75	103	duplicate
4219	35	Pyroglutamic acid	55	[612; 4-Aminobutyric acid (2TBS)]	43	-0.561	-0.914	50.945	0.571	135	6	136	5	131	46	original
13037	35	Pyroglutamic acid	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.569	-0.717	44.229	0.516	136	5	126	15	111	70	duplicate
4213	35	Pyroglutamic acid	49	[877; Pyrophosphoric acid (4TMS)]	64	-0.571	-0.674	56.154	0.488	137	4	125	16	138	86	original
4295	35	Pyroglutamic acid	131	[826; 5-Methylthioadenosine (3TMS)]	55	-0.635	-0.810	50.713	0.588	138	3	131	10	130	35	original
4246	35	Pyroglutamic acid	82	Lysine	39	-0.638	-0.934	25.604	0.660	139	2	138	3	33	5	original
12447	35	Pyroglutamic acid	20	[618; 2-(3',4'-Bishydroxyphenyl)-2-oxethylamine (4TMS)]	31	-0.755	-0.971	37.648	0.657	140	1	140	1	76	6	duplicate
4335	36	N-Acetylglutamic acid	66	Glycine acid-3-phosphate	64	0.481	0.837	28.884	0.515	1	140	1	140	90	20	original
4344	36	N-Acetylglutamic acid	75	Lysine	64	0.457	0.737	12.500	0.543	2	139	4	137	16	8	original
4327	36	N-Acetylglutamic acid	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	0.417	0.623	15.239	0.534	3	138	16	125	29	15	original
13267	36	N-Acetylglutamic acid	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	0.398	0.628	36.996	0.486	4	137	14	127	125	29	duplicate
10255	36	N-Acetylglutamic acid	3	Ethanolamine	62	0.383	0.648	32.826	0.454	5	136	10	131	110	51	duplicate
4350	36	N-Acetylglutamic acid	81	Tyrosine	64	0.379	0.711	8.944	0.549	6	135	6	135	7	6	original
11193	36	N-Acetylglutamic acid	10	Glycine	64	0.370	0.587	12.826	0.436	7	134	21	120	17	63	duplicate
4399	36	N-Acetylglutamic acid	130	Trehalose	63	0.359	0.538	6.192	0.431	8	133	27	114	2	66	original
4328	36	N-Acetylglutamic acid	59	Ornithine; Arginine	64	0.354	0.560	14.191	0.485	9	132	24	117	23	30	original
4336	36	N-Acetylglutamic acid	87	Citric acid	64	0.344	0.643	7.192	0.455	10	131	12	129	4	50	original
4387	36	N-Acetylglutamic acid	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	48	0.340	0.570	38.334	0.465	11	130	23	118	128	41	original
10392	36	N-Acetylglutamic acid	4	Phosphoric acid	51	0.324	0.778	6.465	0.560	12	129	2	139	3	5	duplicate
4329	36	N-Acetylglutamic acid	60	Glyceral-3-phosphate	64	0.318	0.661	8.730	0.535	13	128	9	132	6	14	original
13822	36	N-Acetylglutamic acid	32	[729; N,N-Dimethyllysine methyl ester]	63	0.312	0.646	34.363	0.520	14	127	11	130	117	19	duplicate
13713	36	N-Acetylglutamic acid	31	[622; Perabanic acid (2TMS)]	64	0.311	0.594	33.476	0.483	15	126	20	121	112	31	duplicate
4346	36	N-Acetylglutamic acid	77	[826; beta-[[[5-methyl-2-thienyl)methyl]eneamino- benzeneacetic acid methyl ester]	62	0.304	0.640	10.444	0.504	16	125	13	128	12	24	original
10117	36	N-Acetylglutamic acid	2	Serine	62	0.302	0.709	17.808	0.513	17	124	7	134	43	21	duplicate
11062	36	N-Acetylglutamic acid	9	Proline	63	0.296	0.715	13.044	0.542	18	123	5	136	18	10	duplicate
4352	36	N-Acetylglutamic acid	83	Sorbitol	58	0.286	0.693	10.355	0.568	19	122	8	133	10	2	original
4340	36	N-Acetylglutamic acid	71	[731; Erythrose (3TMS)]	64	0.276	0.599	17.880	0.469	20	121	19	122	44	38	original
4338	36	N-Acetylglutamic acid	69	Arginine	60	0.268	0.538	13.470	0.512	21	120	26	115	21	22	original
4306	36	N-Acetylglutamic acid	37	Phenylalanine	64	0.266	0.625	7.783	0.488	22	119	15	126	5	28	original
4393	36	N-Acetylglutamic acid	124	[734; 1-Monooctadecylglycerol (2TMS); 1- Monohexadecanoylglycerol (1TMS)]	59	0.262	0.458	46.485	0.367	23	118	30	111	140	114	original
4311	36	N-Acetylglutamic acid	42	Glutamic acid	60	0.260	0.599	13.358	0.509	24	117	18	123	20	23	original
10797	36	N-Acetylglutamic acid	7	Threonine	64	0.250	0.605	5.899	0.483	25	116	17	124	1	32	duplicate
4407	36	N-Acetylglutamic acid	138	[674; Ergosterol (1TMS)]	46	0.248	0.474	35.548	0.379	26	115	29	112	121	104	original

4400	36 [596; N-Acetylglutamic ε 131 [626; 5-Methylthiadenosine (3TMS)]	55	0.228	0.197	38.635	0.409	27	114	45	96	129	86 original
12805	36 [596; N-Acetylglutamic ε 23 Homoserine	64	0.226	0.482	25.200	0.444	28	113	28	113	69	56 duplicate
4373	36 [596; N-Acetylglutamic ε 104 [795; Erythritol (4TMS)]	63	0.216	0.296	26.641	0.424	29	112	38	103	79	74 original
4320	36 [596; N-Acetylglutamic ε 51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	0.211	0.551	39.630	0.489	30	111	25	116	131	27 original
4317	36 [596; N-Acetylglutamic ε 48 Asparagine	64	0.211	0.358	26.499	0.432	31	110	34	107	76	65 original
13603	36 [596; N-Acetylglutamic ε 30 [815; Ethyl-3(2H)-thiophenone]	64	0.203	0.396	10.371	0.459	32	109	32	109	11	46 duplicate
4402	36 [596; N-Acetylglutamic ε 133 [855; Squalene]	64	0.199	0.368	25.746	0.384	33	108	33	108	72	102 original
13830	36 [596; N-Acetylglutamic ε 33 Methionine	64	0.197	0.310	25.850	0.420	34	107	37	104	73	76 duplicate
10930	36 [596; N-Acetylglutamic ε 8 Isoleucine	55	0.182	0.752	16.345	0.540	35	106	3	138	34	13 duplicate
4408	36 [596; N-Acetylglutamic ε 137 Ergosterol	64	0.159	0.315	19.687	0.379	36	105	36	105	48	105 original
4348	36 [596; N-Acetylglutamic ε 79 Glucose	64	0.158	0.020	12.404	0.541	37	104	64	77	15	12 original
4333	36 [596; N-Acetylglutamic ε 64 [789; Tyramine (3TMS)]	63	0.152	0.112	27.725	0.329	38	103	51	80	85	135 original
13038	36 [596; N-Acetylglutamic ε 25 [709; 2,5-Diaminovalerolactam (2TMS)]	48	0.151	0.456	29.448	0.399	39	102	31	110	95	88 duplicate
4337	36 [596; N-Acetylglutamic ε 68 [570; Hypoxanthine (2TMS)]	20	0.147	0.586	27.578	0.361	40	101	22	119	83	123 original
4377	36 [596; N-Acetylglutamic ε 108 Octadecenoic acid	64	0.143	0.356	29.655	0.358	41	99	35	106	96	124 original
14037	36 [596; N-Acetylglutamic ε 34 Aspartic acid	64	0.143	0.255	9.845	0.397	42	100	42	99	8	89 duplicate
4363	36 [596; N-Acetylglutamic ε 94 Hexadecanoic acid	64	0.129	0.271	12.281	0.387	43	98	40	101	14	99 original
4392	36 [596; N-Acetylglutamic ε 123 [945; Galactoturanose-6-phosphate (7TMS)]	64	0.128	0.192	20.119	0.467	44	97	46	95	49	40 original
4378	36 [596; N-Acetylglutamic ε 109 Octadecanoic acid	64	0.124	0.265	15.948	0.364	45	96	41	100	32	119 original
4312	36 [596; N-Acetylglutamic ε 43 [548; Leucine (2TBS)]	60	0.120	0.040	24.096	0.350	46	95	61	80	62	127 original
4314	36 [596; N-Acetylglutamic ε 45 Homocysteine	61	0.114	0.043	44.878	0.404	47	94	60	81	139	87 original
12205	36 [596; N-Acetylglutamic ε 18 [590; 1-Acetyl-2-thiohydantoin]	64	0.108	0.052	23.861	0.363	48	93	57	84	61	121 duplicate
4364	36 [596; N-Acetylglutamic ε 95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	0.099	0.291	39.792	0.295	49	92	39	102	132	138 original
12327	36 [596; N-Acetylglutamic ε 19 Alanine (BP) (3TMS)	64	0.096	0.017	20.532	0.413	50	91	66	75	53	82 duplicate
4383	36 [596; N-Acetylglutamic ε 114 Fructose-6-phosphate	53	0.094	-0.038	29.063	0.415	51	90	73	68	91	81 original
4382	36 [596; N-Acetylglutamic ε 113 Galactose-6-phosphate	62	0.082	-0.100	30.830	0.441	52	89	78	63	102	57 original
4410	36 [596; N-Acetylglutamic ε 141 Lanostol-8,24-dien-3-beta-ol	61	0.080	0.144	37.268	0.410	53	88	48	93	126	85 original
4310	36 [596; N-Acetylglutamic ε 41 [638; Proline (2TMS)]	64	0.071	0.079	17.702	0.394	54	87	53	88	42	94 original
4330	36 [596; N-Acetylglutamic ε 61 [NA]	64	0.053	0.078	26.575	0.339	55	86	54	87	78	131 original
11833	36 [596; N-Acetylglutamic ε 15 Alanine	64	0.048	0.049	14.698	0.424	56	85	58	83	26	72 duplicate
4324	36 [596; N-Acetylglutamic ε 55 [612; 4-Aminobutyric acid (2TBS)]	43	0.045	0.135	43.202	0.544	57	84	49	92	138	7 original
4409	36 [596; N-Acetylglutamic ε 140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49	0.043	0.023	37.293	0.393	58	83	63	78	127	96 original
4387	36 [596; N-Acetylglutamic ε 118 [928; Glucopyranose-6-phosphate (6TMS)]	58	0.041	-0.009	29.279	0.318	59	82	69	72	92	136 original
4318	36 [596; N-Acetylglutamic ε 49 [877; Pyrophosphoric acid (4TMS)]	64	0.036	0.010	42.747	0.367	60	81	67	74	136	115 original
4351	36 [596; N-Acetylglutamic ε 82 Lysine	39	0.031	0.073	17.680	0.541	61	80	56	85	41	11 original
4321	36 [596; N-Acetylglutamic ε 52 [NA]	46	0.024	0.126	36.722	0.478	62	79	50	91	124	34 original
4358	36 [596; N-Acetylglutamic ε 89 [775; Dopamine (4TMS)]	35	0.015	0.248	29.827	0.463	63	78	43	98	97	45 original
10528	36 [596; N-Acetylglutamic ε 5 Leucine	45	0.012	0.207	29.311	0.561	64	77	44	97	93	4 duplicate
4395	36 [596; N-Acetylglutamic ε 128 [559; Erythritol (4TMS)]	45	0.008	0.086	24.819	0.468	65	76	52	89	66	39 original
4408	36 [596; N-Acetylglutamic ε 139 [700; Ergosta-5,7-dien-3-ol]	38	0.007	-0.025	36.260	0.301	66	75	71	70	123	137 original
4380	36 [596; N-Acetylglutamic ε 111 [583; Erythritol (4TMS)]	42	0.006	0.036	38.855	0.278	67	74	62	79	130	139 original
4388	36 [596; N-Acetylglutamic ε 119 [931; myo-Inositol-2-phosphate (7TMS)]	64	0.003	-0.007	25.521	0.354	68	73	68	73	71	128 original
4354	36 [596; N-Acetylglutamic ε 85 [528; Methylcitric acid (4TMS)]	48	-0.005	-0.055	26.021	0.568	69	72	74	67	75	1 original
4376	36 [596; N-Acetylglutamic ε 107 9-(Z)-Octadecenoic acid	64	-0.019	0.043	16.245	0.348	70	71	59	82	33	129 original
4313	36 [596; N-Acetylglutamic ε 44 [910; 2-Ketogluconic acid methoxamine (4TMS)]	50	-0.024	-0.079	22.921	0.450	71	70	75	66	59	52 original
12448	36 [596; N-Acetylglutamic ε 20 [619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.037	0.020	32.423	0.528	72	69	65	76	107	17 duplicate
4386	36 [596; N-Acetylglutamic ε 117 [724; Glycerol (3TMS)]	56	-0.040	-0.119	27.866	0.418	73	68	79	62	86	77 original
4391	36 [596; N-Acetylglutamic ε 122 [644; Erythritol (4TMS)]	52	-0.042	-0.199	35.608	0.458	74	67	85	56	122	47 original
4341	36 [596; N-Acetylglutamic ε 72 [919; D-Xylopyranose (4TMS)]	63	-0.046	-0.089	30.889	0.338	75	66	76	65	103	132 original
12568	36 [596; N-Acetylglutamic ε 21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	-0.049	-0.278	15.181	0.446	76	65	94	47	28	55 duplicate

4342	36 [596; N-Acetylglycamic $\epsilon$ 73 [708; Glucose methoxyamine (5TMS)]	57	-0.049	-0.130	31.529	0.396	77	64	81	60	105	92 original
4343	36 [596; N-Acetylglycamic $\epsilon$ 74 [912; Tetradecanoic acid (1TMS)]	64	-0.050	-0.022	30.391	0.394	78	63	70	71	100	93 original
10663	36 [596; N-Acetylglycamic $\epsilon$ 6 Glycerol	64	-0.063	-0.200	16.480	0.374	79	62	88	55	35	109 duplicate
4339	36 [596; N-Acetylglycamic $\epsilon$ 70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	-0.070	-0.092	14.301	0.386	80	61	77	64	24	101 original
4332	36 [596; N-Acetylglycamic $\epsilon$ 63 Glutamine	52	-0.072	0.187	30.680	0.344	81	60	47	94	101	130 original
4390	36 [596; N-Acetylglycamic $\epsilon$ 121 [657; Erythritol (4TMS)]	55	-0.077	-0.034	35.322	0.410	82	59	72	69	120	84 original
4405	36 [596; N-Acetylglycamic $\epsilon$ 136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.088	0.078	13.214	0.332	83	58	55	86	19	134 original
4322	36 [596; N-Acetylglycamic $\epsilon$ 53 Glycerol-2-phosphate	64	-0.092	-0.228	34.989	0.370	84	57	88	53	118	113 original
4379	36 [596; N-Acetylglycamic $\epsilon$ 110 [715; Erythritol (4TMS)]	54	-0.106	-0.183	30.914	0.568	85	56	83	58	104	3 original
4347	36 [596; N-Acetylglycamic $\epsilon$ 78 Mannose	62	-0.107	-0.185	32.584	0.418	86	55	84	57	108	78 original
4375	36 [596; N-Acetylglycamic $\epsilon$ 106 [733; Threitol (4TMS)]	62	-0.108	-0.201	25.865	0.503	87	54	87	54	74	25 original
4389	36 [596; N-Acetylglycamic $\epsilon$ 120 [945; Uridine (3TMS)]	54	-0.115	-0.128	17.166	0.392	88	53	80	61	38	103 original
4384	36 [596; N-Acetylglycamic $\epsilon$ 115 Glucose-6-phosphate	62	-0.118	-0.259	11.709	0.377	89	52	91	50	13	106 original
4394	36 [596; N-Acetylglycamic $\epsilon$ 125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	-0.118	-0.289	15.036	0.362	90	51	96	45	27	122 original
4309	36 [596; N-Acetylglycamic $\epsilon$ 40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.121	-0.233	10.057	0.458	91	50	90	51	9	48 original
4345	36 [596; N-Acetylglycamic $\epsilon$ 76 Fructose	64	-0.123	-0.295	15.867	0.371	92	49	98	43	31	112 original
14143	36 [596; N-Acetylglycamic $\epsilon$ 35 Pyroglutamic acid	64	-0.131	-0.315	16.562	0.396	93	48	99	42	38	90 duplicate
4349	36 [596; N-Acetylglycamic $\epsilon$ 80 [772; D-Glucose (5TMS)]	62	-0.132	-0.281	15.446	0.365	94	47	95	46	30	116 original
4365	36 [596; N-Acetylglycamic $\epsilon$ 98 myo-Inositol	49	-0.141	-0.130	41.338	0.394	95	46	82	59	135	118 original
4369	36 [596; N-Acetylglycamic $\epsilon$ 100 [857; Mannitol (6TMS)]	64	-0.184	-0.366	22.862	0.396	96	45	103	38	58	91 original
4359	36 [596; N-Acetylglycamic $\epsilon$ 90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	64	-0.186	-0.266	25.312	0.385	97	44	92	49	70	117 original
4401	36 [596; N-Acetylglycamic $\epsilon$ 132 [895; Isomaltose methoxyamine (8TMS)]	42	-0.187	-0.451	32.825	0.332	98	43	106	35	109	133 original
4371	36 [596; N-Acetylglycamic $\epsilon$ 102 [904; Galactose methoxyamine (5TMS)]	64	-0.189	-0.292	29.904	0.364	99	42	97	44	98	120 original
13153	36 [596; N-Acetylglycamic $\epsilon$ 26 Citramalic acid	64	-0.198	-0.360	14.419	0.374	100	41	100	41	25	108 duplicate
13380	36 [596; N-Acetylglycamic $\epsilon$ 28 Malic acid	64	-0.206	-0.472	22.275	0.424	101	40	108	33	55	71 duplicate
4385	36 [596; N-Acetylglycamic $\epsilon$ 116 [882; Pseudouridine (5TMS)]	30	-0.214	-0.231	24.381	0.500	102	39	89	52	64	26 original
4404	36 [596; N-Acetylglycamic $\epsilon$ 902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	-0.230	-0.273	18.299	0.376	103	38	93	48	47	107 original
4398	36 [596; N-Acetylglycamic $\epsilon$ 127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	39	-0.244	-0.364	20.294	0.218	104	37	102	39	51	140 original
4356	36 [596; N-Acetylglycamic $\epsilon$ 87 [945; beta-D-Glucopyranose (5TMS)]	62	-0.253	-0.361	17.261	0.373	105	36	101	40	39	110 original
11707	36 [596; N-Acetylglycamic $\epsilon$ 14 Fumaric acid	64	-0.258	-0.507	33.324	0.425	106	35	110	31	111	70 duplicate
4381	36 [596; N-Acetylglycamic $\epsilon$ 112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	-0.261	-0.367	40.848	0.412	107	34	104	37	134	83 original
4307	36 [596; N-Acetylglycamic $\epsilon$ 38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.275	-0.544	25.109	0.436	108	33	113	28	68	62 original
4331	36 [596; N-Acetylglycamic $\epsilon$ 62 [812; D-Xylofuranose (4TMS)]	64	-0.277	-0.489	17.516	0.440	109	32	109	32	40	58 original
4355	36 [596; N-Acetylglycamic $\epsilon$ 86 [793; D-Galactono-1,4-lactone (4TMS)]	61	-0.289	-0.469	27.208	0.438	110	31	107	34	82	59 original
12687	36 [596; N-Acetylglycamic $\epsilon$ 22 [690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	52	-0.297	-0.571	33.806	0.389	111	30	118	23	115	98 duplicate
4353	36 [596; N-Acetylglycamic $\epsilon$ 84 Mannitol	62	-0.321	-0.838	18.026	0.542	112	29	140	1	46	9 original
4308	36 [596; N-Acetylglycamic $\epsilon$ 39 [829; 1-Phenylethanol (1TMS)]	63	-0.328	-0.574	24.238	0.424	113	28	119	22	63	73 original
11323	36 [596; N-Acetylglycamic $\epsilon$ 11 Succinic acid	64	-0.343	-0.543	24.394	0.424	114	27	112	29	65	75 duplicate
4357	36 [596; N-Acetylglycamic $\epsilon$ 88 Gluconic acid	64	-0.344	-0.627	24.933	0.470	115	26	129	12	67	37 original
4316	36 [596; N-Acetylglycamic $\epsilon$ 47 [NA]	64	-0.354	-0.560	29.370	0.463	116	25	115	26	94	44 original
11452	36 [596; N-Acetylglycamic $\epsilon$ 128 Glycetic acid	63	-0.359	-0.575	35.286	0.417	117	24	120	21	119	80 duplicate
4397	36 [596; N-Acetylglycamic $\epsilon$ 12 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45	-0.360	-0.526	20.795	0.372	118	23	111	30	54	111 original
4319	36 [596; N-Acetylglycamic $\epsilon$ 50 [746; Ribonic acid-1,4-lactone (3TMS)]	61	-0.363	-0.607	42.850	0.450	119	22	126	15	137	53 original
4370	36 [596; N-Acetylglycamic $\epsilon$ 101 [832; Dopamine (4TMS)]	64	-0.367	-0.728	28.485	0.470	120	21	137	4	88	36 original
13492	36 [596; N-Acetylglycamic $\epsilon$ 29 Erythritol	64	-0.368	-0.616	28.116	0.457	121	20	128	13	87	49 duplicate
4372	36 [596; N-Acetylglycamic $\epsilon$ 103 [648; Ethylamine (2TMS)]	63	-0.368	-0.722	28.659	0.480	122	19	135	6	89	33 original
4361	36 [596; N-Acetylglycamic $\epsilon$ 92 [680; Glycero-2-phosphate (4TMS)]	54	-0.377	-0.387	26.977	0.349	123	18	105	36	81	128 original
12922	36 [596; N-Acetylglycamic $\epsilon$ 24 [725; 2-Ketocacetic acid (2TMS)]	64	-0.385	-0.612	13.885	0.448	124	17	127	14	22	54 duplicate
4360	36 [596; N-Acetylglycamic $\epsilon$ 91 [766; beta-D-Methylglucopyranoside (4TMS)]	64	-0.387	-0.803	31.998	0.522	125	16	139	2	106	18 original
11958	36 [596; N-Acetylglycamic $\epsilon$ 16 [644; 2-Methyl-1,3-butanediol (2TMS)]	64	-0.391	-0.635	16.605	0.463	126	15	130	11	37	42 duplicate

4315	36 [596; N-Acetylglutamic ε 46	Arabinose	64 -0.396	-0.566	26.677	0.427	127	13	117	24	80	68 original
12082	38 [596; N-Acetylglutamic ε 17	[700; 2-methyl-1,2-propanediol (2TMS)]	64 -0.396	-0.595	17.921	0.436	128	14	123	18	45	64 duplicate
4403	36 [596; N-Acetylglutamic ε 134	Isomaltose	64 -0.397	-0.588	20.434	0.438	129	12	121	20	52	60 original
4334	38 [596; N-Acetylglutamic ε 65	[646; 3-Deoxyglucitol (5TMS)]	63 -0.402	-0.565	34.305	0.426	130	11	116	25	116	69 original
4362	36 [596; N-Acetylglutamic ε 93	[607; Putrescine (4TMS)]	60 -0.406	-0.692	40.162	0.474	131	10	133	8	133	35 original
11580	36 [596; N-Acetylglutamic ε 13	Uracil	64 -0.409	-0.644	20.123	0.463	132	9	132	9	50	43 duplicate
4325	36 [596; N-Acetylglutamic ε 56	[829; Orolic acid (3TMS)]	64 -0.424	-0.597	33.607	0.428	133	8	125	16	113	67 original
4398	36 [596; N-Acetylglutamic ε 129	[840; Maltose methoxymine (6TMS); alpha-D-Glc-(1,4)-D-Glc]	59 -0.430	-0.593	29.988	0.387	134	7	122	19	99	100 original
4368	36 [596; N-Acetylglutamic ε 99	[662; Ribose-5-phosphate methoxymine (BP) (5TMS)]	41 -0.441	-0.596	27.717	0.365	135	6	124	17	84	125 original
4366	36 [596; N-Acetylglutamic ε 97	[756; beta-D-Methylglucopyranoside (4TMS)]	52 -0.448	-0.700	22.409	0.530	136	5	134	7	57	18 original
4374	36 [596; N-Acetylglutamic ε 105	[705; 2-Ketogluconic acid (5TMS)]	48 -0.473	-0.726	23.524	0.437	137	4	136	5	60	61 original
4323	36 [596; N-Acetylglutamic ε 54	[NA]	55 -0.479	-0.637	33.655	0.393	138	3	131	10	114	85 original
4326	36 [596; N-Acetylglutamic ε 1	[757; 2-Deoxy-pentob-3-yose dimethoxymine (2TMS)]	55 -0.481	-0.557	26.527	0.393	139	2	114	27	77	97 original
9978	36 [596; N-Acetylglutamic ε 81	Tyrosine	36 -0.587	-0.747	22.300	0.417	140	1	138	3	56	79 duplicate
4454	37 Phenylalanine	[570; Hypoxanthine (2TMS)]	64 0.720	0.886	13.089	0.568	1	140	2	139	30	4 original
4441	37 Phenylalanine	[826; beta-[[[5-methyl-2-thienyl]methyl]eneamino-benzeneacetic acid methyl ester]	20 0.716	0.811	24.797	0.545	2	139	9	132	88	8 original
4450	37 Phenylalanine	Citric acid	62 0.712	0.902	11.736	0.576	3	138	1	140	24	2 original
4440	37 Phenylalanine	[815; Ethyl-3-(2H)-thiophenone]	64 0.695	0.836	2.011	0.533	4	137	7	134	1	13 original
13604	37 Phenylalanine	Glycerol-3-phosphate	64 0.684	0.765	10.494	0.514	5	136	14	127	18	21 duplicate
4433	37 Phenylalanine	Ethanolamine	64 0.680	0.855	2.747	0.565	6	135	3	136	2	6 original
10266	37 Phenylalanine	Glutamic acid	62 0.662	0.822	27.304	0.541	7	134	8	133	109	11 duplicate
4415	37 Phenylalanine	Threonine	60 0.636	0.846	14.231	0.535	8	133	5	136	37	12 original
10798	37 Phenylalanine	Methionine	64 0.635	0.855	7.830	0.515	9	132	4	137	5	19 duplicate
13931	37 Phenylalanine	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	64 0.622	0.725	19.913	0.461	10	131	18	123	70	62 duplicate
4424	37 Phenylalanine	Ornithine; Arginine	44 0.600	0.798	35.101	0.572	11	130	11	130	134	3 original
4432	37 Phenylalanine	Arginine	64 0.600	0.792	18.764	0.495	12	129	12	129	64	32 original
4442	37 Phenylalanine	Glycine	60 0.598	0.764	10.304	0.542	13	128	15	126	15	10 original
11194	37 Phenylalanine	[729; N,N-Dimethyllysine methyl ester]	64 0.594	0.743	8.146	0.500	14	127	16	125	7	30 duplicate
13823	37 Phenylalanine	Proline	63 0.560	0.845	29.391	0.544	15	126	6	135	119	9 duplicate
11063	37 Phenylalanine	Aspartic acid	63 0.559	0.811	13.731	0.483	16	125	10	131	35	42 duplicate
13714	37 Phenylalanine	[622; Perabanic acid (2TMS)]	64 0.536	0.657	11.455	0.440	17	124	22	119	21	82 duplicate
4428	37 Phenylalanine	[612; 4-Aminobutyric acid (2TBS)]	43 0.530	0.645	37.122	0.532	19	122	19	122	113	57 duplicate
10931	37 Phenylalanine	Isolaucine	55 0.518	0.689	13.439	0.455	20	121	20	121	33	14 original
4421	37 Phenylalanine	Asparagine	64 0.505	0.635	20.917	0.493	21	120	26	115	77	68 duplicate
4444	37 Phenylalanine	[731; Erythrose (3TMS)]	64 0.494	0.643	11.637	0.456	22	119	25	116	22	34 original
10118	37 Phenylalanine	Serine	62 0.479	0.790	14.786	0.527	23	118	13	128	41	67 original
4455	37 Phenylalanine	Lysine	39 0.471	0.656	13.098	0.551	24	117	23	118	31	15 duplicate
10529	37 Phenylalanine	Leucine	45 0.467	0.600	23.112	0.505	25	116	28	113	88	7 original
4468	37 Phenylalanine	[770; 3,4,6-Trisidhydroxyphenylethanolamine (5TMS)]	50 0.464	0.552	35.074	0.374	26	115	33	108	133	27 duplicate
4434	37 Phenylalanine	[NA]	64 0.455	0.508	20.268	0.423	27	114	35	106	73	125 original
4418	37 Phenylalanine	Homocysteine	61 0.454	0.487	39.322	0.413	28	113	36	105	139	88 original
4439	37 Phenylalanine	Glyceric acid-3-phosphate	64 0.451	0.729	23.159	0.473	29	112	37	124	90	102 original
12806	37 Phenylalanine	Homoserine	64 0.413	0.594	19.847	0.473	30	111	29	112	69	50 original
4509	37 Phenylalanine	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17 0.397	0.472	10.406	0.273	31	110	39	102	16	49 duplicate
4471	37 Phenylalanine	[697; Ribose-5-phosphate methoxymine (5TMS)]	48 0.394	0.578	33.702	0.449	32	109	31	110	129	140 original
4462	37 Phenylalanine	[775; Dopamine (4TMS)]	35 0.375	0.465	26.287	0.508	33	108	40	101	108	71 original
4504	37 Phenylalanine	[626; 5-Methylthioadenosine (3TMS)]	55 0.333	0.302	32.835	0.463	34	107	51	90	128	25 original



4481	37 Phenylalanine	108 Octadecanoic acid	64	0.310	0.456	23,750	0.365	35	108	42	99	83	129 original
4425	37 Phenylalanine	52 [NA]	46	0.300	0.441	32,580	0.565	36	105	44	97	127	5 original
4484	37 Phenylalanine	111 [593; Erythritol (4TMS)]	42	0.288	0.325	34,148	0.321	37	104	50	91	131	137 original
13268	37 Phenylalanine	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	0.287	0.588	32,369	0.505	38	103	30	111	126	28 duplicate
4448	37 Phenylalanine	75 Lysine	64	0.267	0.688	17,616	0.525	39	102	21	120	52	16 original
14249	37 Phenylalanine	36 [596; N-Acetylglutamic acid (2TMS)]	64	0.266	0.625	7,793	0.488	40	101	27	114	3	36 duplicate
4497	37 Phenylalanine	124 [734; 1-Monoleoylglycerol (2TMS); 1-Monoheptadecanoylglycerol (1TMS)]	59	0.264	0.428	41,050	0.376	41	100	45	98	140	122 original
4510	37 Phenylalanine	137 Ergosterol	64	0.262	0.478	14,281	0.365	42	99	37	104	40	130 original
4422	37 Phenylalanine	49 [877; Pyrophosphoric acid (4TMS)]	64	0.236	0.229	36,861	0.375	43	98	55	86	136	123 original
4456	37 Phenylalanine	85 Sorbitol	58	0.230	0.474	7,851	0.477	44	97	38	103	6	48 original
13039	37 Phenylalanine	25 [709; 2,5-Diaminovalerolactam (2TMS)]	48	0.216	0.517	25,661	0.432	45	98	34	107	103	83 duplicate
4480	37 Phenylalanine	107 9-(Z)-Octadecanoic acid	64	0.209	0.327	9,650	0.361	46	95	49	92	12	133 original
12449	37 Phenylalanine	20 [819; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	0.204	0.465	27,526	0.577	47	94	41	100	111	1 duplicate
4511	37 Phenylalanine	138 [674; Ergosterol (1TMS)]	46	0.200	0.391	31,191	0.408	48	93	47	94	122	108 original
4492	37 Phenylalanine	119 [931; myo-Inositol-2-phosphate (7TMS)]	64	0.199	0.269	19,266	0.405	49	92	53	88	68	111 original
4467	37 Phenylalanine	94 Hexadecanoic acid	64	0.177	0.244	8,652	0.406	50	91	54	87	9	109 original
4436	37 Phenylalanine	63 Glutamine	52	0.173	0.442	26,285	0.460	51	90	43	98	105	63 original
4431	37 Phenylalanine	58 [636; 4R-Acetalamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	0.155	0.575	10,481	0.480	52	89	32	109	17	44 original
4482	37 Phenylalanine	109 Octadecanoic acid	64	0.152	0.161	13,386	0.320	53	88	59	82	32	138 original
4514	37 Phenylalanine	141 Lanosta-8,24-dien-3-beta-ol	61	0.136	0.167	31,438	0.401	54	87	58	83	123	113 original
4416	37 Phenylalanine	43 [548; Leucine (2TBS)]	60	0.130	0.207	18,268	0.368	55	88	57	84	59	127 original
4506	37 Phenylalanine	133 [855; Squalene]	64	0.124	0.371	20,020	0.414	56	85	48	93	71	98 original
4512	37 Phenylalanine	139 [700; Ergosta-5,7-dien-3-ol]	38	0.115	0.215	31,859	0.369	57	84	56	85	125	126 original
4503	37 Phenylalanine	130 Trehalose	63	0.099	0.269	8,393	0.379	58	83	52	89	8	120 original
4437	37 Phenylalanine	64 [789; Tyramine (3TMS)]	63	0.070	0.069	21,731	0.375	59	82	61	80	82	124 original
4489	37 Phenylalanine	116 [882; Pseudouridine (5TMS)]	30	0.044	0.094	19,584	0.449	60	81	60	81	68	72 original
10393	37 Phenylalanine	4 Phosphoric acid	51	0.034	0.409	12,799	0.467	61	80	46	95	28	56 duplicate
4508	37 Phenylalanine	135 [902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	0.026	-0.040	11,719	0.358	62	79	66	75	23	134 original
4463	37 Phenylalanine	90 [910; 9-(Z)-Hexadecanoic acid (1TMS)]	64	0.021	0.009	18,881	0.377	63	78	64	77	65	121 original
4469	37 Phenylalanine	96 myo-Inositol	49	0.009	-0.005	35,823	0.363	64	77	65	76	135	132 original
11834	37 Phenylalanine	15 Alanine	64	0.008	-0.109	9,802	0.481	65	76	69	72	14	43 duplicate
4513	37 Phenylalanine	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49	0.007	0.013	31,925	0.408	66	75	63	78	124	105 original
4496	37 Phenylalanine	123 [945; Galactofuranose-6-phosphate (7TMS)]	64	-0.011	-0.074	14,244	0.493	67	74	67	74	39	33 original
4499	37 Phenylalanine	126 [559; Erythritol (4TMS)]	45	-0.018	0.031	20,310	0.452	68	73	62	79	74	69 original
4458	37 Phenylalanine	85 [529; Methyldiciric acid (4TMS)]	48	-0.039	-0.120	19,331	0.487	69	72	70	71	67	39 original
4486	37 Phenylalanine	113 Galactose-6-phosphate	62	-0.049	-0.319	25,240	0.487	70	71	86	55	100	38 original
4487	37 Phenylalanine	114 Fructose-6-phosphate	53	-0.051	-0.254	24,341	0.496	71	70	78	63	96	31 original
4475	37 Phenylalanine	102 [904; Galactose methoxamine (5TMS)]	64	-0.059	-0.147	23,873	0.414	72	69	73	68	92	99 original
4466	37 Phenylalanine	93 [607; Putrescine (4TMS)]	60	-0.076	-0.372	33,911	0.446	73	68	88	53	130	75 original
4457	37 Phenylalanine	84 Mannitol	62	-0.086	-0.612	15,776	0.515	74	67	113	28	47	20 original
4485	37 Phenylalanine	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	-0.087	-0.192	34,952	0.422	75	66	75	66	132	92 original
4500	37 Phenylalanine	127 [777; Fructose-6-phosphate methoxamine (6TMS)]	39	-0.104	-0.292	15,920	0.307	76	65	82	59	49	139 original
4505	37 Phenylalanine	132 [895; Isomaltose methoxamine (6TMS)]	42	-0.110	-0.502	28,331	0.348	77	64	100	41	114	135 original
4452	37 Phenylalanine	79 Glucose	64	-0.114	-0.317	15,272	0.463	78	63	85	56	43	60 original
4447	37 Phenylalanine	74 [912; Tetradecanoic acid (1TMS)]	64	-0.115	-0.097	24,719	0.427	79	62	68	73	97	84 original
4473	37 Phenylalanine	100 [857; Mannitol (6TMS)]	64	-0.122	-0.309	16,466	0.392	80	61	84	57	50	115 original
12206	37 Phenylalanine	18 [590; 1-Acetyl-2-thiohydantoin]	64	-0.134	-0.130	17,838	0.348	81	60	71	70	54	136 duplicate

4445	37 Phenylalanine	72 [919; D-Xylopyranose (4TMS)]	63 -0.146	-0.187	25.012	0.382	82	59	74	67	99	119 original
4417	37 Phenylalanine	44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	50 -0.159	-0.226	18.032	0.426	83	58	76	65	57	86 original
4491	37 Phenylalanine	118 [928; Glucopyranose-6-phosphate (6TMS)]	58 -0.162	-0.284	24.060	0.390	84	57	78	62	94	117 original
4426	37 Phenylalanine	53 Glycerol-2-phosphate	64 -0.172	-0.265	28.915	0.363	85	56	81	60	117	131 original
4414	37 Phenylalanine	41 [639; Proline (2TMS)]	64 -0.173	-0.136	11.929	0.488	86	55	72	69	25	37 original
4477	37 Phenylalanine	104 [795; Erythritol (4TMS)]	63 -0.184	-0.254	21.446	0.457	87	54	77	64	80	66 original
12328	37 Phenylalanine	19 Alanine (BP) (3TMS)	64 -0.207	-0.268	14.977	0.483	88	53	80	61	42	41 duplicate
14144	37 Phenylalanine	35 Pyroglutamic acid	64 -0.214	-0.489	20.152	0.445	89	52	89	42	72	78 duplicate
4488	37 Phenylalanine	115 Glucose-6-phosphate	62 -0.236	-0.447	9.144	0.422	90	51	98	45	11	89 original
13381	37 Phenylalanine	28 Malic acid	64 -0.242	-0.510	15.876	0.442	91	50	101	40	48	81 duplicate
4501	37 Phenylalanine	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45 -0.253	-0.410	15.346	0.413	92	49	95	46	44	101 original
4495	37 Phenylalanine	122 [644; Erythritol (4TMS)]	52 -0.263	-0.392	30.573	0.412	93	48	92	49	121	104 original
11453	37 Phenylalanine	12 Glycine acid	63 -0.263	-0.524	29.155	0.422	94	47	103	38	118	90 duplicate
13154	37 Phenylalanine	26 Citramalic acid	64 -0.270	-0.390	7.808	0.397	95	46	91	50	4	114 duplicate
4484	37 Phenylalanine	73 [708; Glucose methoxyamine (5TMS)]	57 -0.278	-0.365	25.622	0.402	96	45	87	54	102	112 original
4483	37 Phenylalanine	121 [657; Erythritol (4TMS)]	55 -0.279	-0.309	30.208	0.391	97	44	83	58	120	116 original
12569	37 Phenylalanine	110 [715; Erythritol (4TMS)]	54 -0.286	-0.392	25.688	0.464	98	43	93	48	104	58 original
4413	37 Phenylalanine	21 [678; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	64 -0.313	-0.460	9.126	0.427	99	42	88	43	10	85 duplicate
11708	37 Phenylalanine	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	64 -0.321	-0.452	12.862	0.417	100	40	97	44	29	97 original
4490	37 Phenylalanine	14 Fumaric acid	64 -0.321	-0.561	27.145	0.449	101	41	109	32	108	73 duplicate
4449	37 Phenylalanine	117 [724; Glycerol (3TMS)]	56 -0.323	-0.397	22.809	0.406	102	39	94	47	86	108 original
4498	37 Phenylalanine	78 Fructose	64 -0.335	-0.553	13.528	0.420	103	38	106	35	34	94 original
4493	37 Phenylalanine	125 [692; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64 -0.346	-0.568	15.398	0.424	104	37	110	31	45	87 original
4451	37 Phenylalanine	120 [945; Uridine (3TMS)]	54 -0.350	-0.385	12.056	0.469	105	36	90	51	26	54 original
11324	37 Phenylalanine	78 Mannose	62 -0.357	-0.521	27.115	0.419	106	35	102	39	107	95 original
4411	37 Phenylalanine	11 Succinic acid	64 -0.357	-0.542	17.987	0.414	107	34	105	36	55	100 duplicate
12688	37 Phenylalanine	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	64 -0.364	-0.623	18.766	0.446	108	33	115	26	63	76 original
4443	37 Phenylalanine	22 [690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	52 -0.371	-0.579	28.642	0.408	109	32	111	30	116	107 duplicate
10664	37 Phenylalanine	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57 -0.373	-0.376	9.746	0.405	110	31	89	52	13	110 original
13493	37 Phenylalanine	6 Glyceral	64 -0.380	-0.556	20.476	0.448	111	30	108	33	75	74 duplicate
4465	37 Phenylalanine	29 Erythritol	64 -0.388	-0.658	21.811	0.468	112	29	118	23	83	55 duplicate
4427	37 Phenylalanine	92 [680; Glycerol-2-phosphate (4TMS)]	54 -0.395	-0.555	21.535	0.366	113	28	107	34	81	128 original
4479	37 Phenylalanine	54 [NA]	55 -0.401	-0.616	27.689	0.384	114	27	114	27	112	118 original
9979	37 Phenylalanine	106 [733; Threitol (4TMS)]	62 -0.421	-0.534	20.706	0.507	115	26	104	37	76	26 original
4435	37 Phenylalanine	1 [938; Sulfuric acid (2TMS)]	38 -0.432	-0.676	18.081	0.422	116	25	121	20	58	93 duplicate
4478	37 Phenylalanine	62 [812; D-Xylofuranose (4TMS)]	64 -0.436	-0.626	11.139	0.444	117	24	116	25	20	79 original
4420	37 Phenylalanine	105 [705; 2-Ketogluconic acid (5TMS)]	48 -0.438	-0.682	17.739	0.418	118	23	124	17	53	96 original
12923	37 Phenylalanine	47 [NA]	64 -0.443	-0.588	23.116	0.422	119	22	112	29	89	91 original
4464	37 Phenylalanine	24 [725; 2-Ketooctanoic acid (2TMS)]	64 -0.464	-0.729	13.776	0.504	120	21	135	6	36	29 duplicate
11959	37 Phenylalanine	91 [766; beta-D-Methylglucopyranoside (4TMS)]	64 -0.466	-0.722	25.581	0.469	121	20	131	10	101	53 original
12083	37 Phenylalanine	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	64 -0.470	-0.723	10.657	0.513	122	19	132	9	19	22 duplicate
4470	37 Phenylalanine	17 [700; 2-methyl-1,2-propanediol (2TMS)]	64 -0.477	-0.682	12.140	0.471	123	18	123	18	27	52 duplicate
4429	37 Phenylalanine	77 [756; beta-D-Methylglucopyranoside (4TMS)]	52 -0.481	-0.757	18.017	0.521	124	17	139	2	56	17 original
4459	37 Phenylalanine	56 [829; Orotic acid (3TMS)]	64 -0.489	-0.719	27.448	0.485	125	16	130	11	110	40 original
4461	37 Phenylalanine	88 [793; D-Galactono-1,4-lactone (4TMS)]	61 -0.490	-0.693	22.966	0.471	126	15	125	16	87	51 original
		57 Gluconic acid	64 -0.491	-0.678	18.688	0.516	127	14	122	19	61	18 original
4430	37 Phenylalanine		55 -0.502	-0.693	21.185	0.446	128	13	126	15	76	77 original
4472	37 Phenylalanine	99 [757; 2-Desoxy-pentos-3-yose dimethoxyamine (2TMS)]	41 -0.502	-0.674	23.546	0.451	129	12	120	21	91	70 original
4453	37 Phenylalanine	80 [772; D-Glucose (5TMS)]	62 -0.503	-0.628	15.460	0.412	130	11	117	24	46	103 original
4476	37 Phenylalanine	103 [648; Ethylamine (2TMS)]	63 -0.503	-0.716	22.465	0.463	131	10	129	12	85	59 original

4507	37	Phenylalanine	134	Isomaltose	64	-0.506	-0.727	16.818	0.477	132	9	134	7	51	45 original
4412	37	Phenylalanine	39	[829; 1-Phenylethanol (1TMS)]	63	-0.508	-0.698	18.734	0.444	133	8	127	14	62	80 original
4474	37	Phenylalanine	101	[832; Dopamine (4TMS)]	64	-0.520	-0.729	22.028	0.459	134	7	136	5	84	64 original
4419	37	Phenylalanine	46	Arabinose	64	-0.525	-0.725	21.369	0.475	135	6	133	8	79	47 original
4438	37	Phenylalanine	65	[646; 3-Deoxyglucitol (5TMS)]	63	-0.538	-0.709	28.404	0.512	136	5	128	13	115	24 original
11581	37	Phenylalanine	13	Uracil	64	-0.556	-0.755	14.238	0.513	137	4	138	3	38	23 duplicate
4502	37	Phenylalanine	129	[840; Maltose methoxyamine (6TMS); alpha-D-Glc-(1,4)-D-Glc]	59	-0.565	-0.732	24.315	0.493	138	3	137	4	95	35 original
4423	37	Phenylalanine	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	-0.576	-0.766	36.968	0.474	139	2	140	1	137	48 original
4460	37	Phenylalanine	87	[945; beta-D-Glucopyranose (5TMS)]	62	-0.583	-0.871	18.478	0.458	140	1	119	22	60	65 original
13494	38	[708; 2,3-Dimethylsuccin	29	Erythritol	64	0.794	0.974	4.208	0.671	1	140	3	138	6	8 duplicate
12924	38	[708; 2,3-Dimethylsuccin	24	[725; 2-Ketooctanoic acid (2TMS)]	64	0.793	0.976	26.631	0.682	2	139	1	140	125	2 duplicate
11960	38	[708; 2,3-Dimethylsuccin	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	0.793	0.978	11.754	0.693	3	138	2	139	60	1 duplicate
4562	38	[708; 2,3-Dimethylsuccin	86	[793; D-Galactono-1,4-lactone (4TMS)]	61	0.751	0.916	17.078	0.672	4	137	20	121	84	7 original
4541	38	[708; 2,3-Dimethylsuccin	65	[646; 3-Deoxyglucitol (5TMS)]	63	0.744	0.981	11.499	0.667	5	136	6	135	58	9 original
11325	38	[708; 2,3-Dimethylsuccin	11	Succinic acid	64	0.743	0.931	1.915	0.630	6	135	18	123	1	26 duplicate
4522	38	[708; 2,3-Dimethylsuccin	46	Arabinose	64	0.738	0.939	12.268	0.661	7	134	14	127	63	14 original
4532	38	[708; 2,3-Dimethylsuccin	56	[829; Orolic acid (3TMS)]	64	0.722	0.942	9.456	0.662	8	133	11	130	42	3 original
4515	38	[708; 2,3-Dimethylsuccin	39	[829; 1-Phenylethanol (1TMS)]	63	0.714	0.972	10.377	0.666	9	132	4	137	48	10 original
4610	38	[708; 2,3-Dimethylsuccin	134	Isomaltose	64	0.711	0.956	19.223	0.674	10	131	8	133	102	6 original
4533	38	[708; 2,3-Dimethylsuccin	57	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55	0.708	0.908	10.152	0.641	11	130	21	120	46	22 original
4526	38	[708; 2,3-Dimethylsuccin	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	0.698	0.938	19.610	0.634	12	129	15	126	105	25 original
11582	38	[708; 2,3-Dimethylsuccin	13	Uracil	64	0.691	0.961	9.975	0.678	13	128	5	138	44	5 duplicate
11709	38	[708; 2,3-Dimethylsuccin	14	Fumaric acid	64	0.689	0.950	9.261	0.644	14	127	9	132	39	20 duplicate
12084	38	[708; 2,3-Dimethylsuccin	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	0.688	0.918	11.586	0.593	15	126	19	122	59	46 duplicate
13382	38	[708; 2,3-Dimethylsuccin	28	Malic acid	64	0.684	0.960	3.094	0.663	16	125	7	134	3	12 duplicate
11454	38	[708; 2,3-Dimethylsuccin	12	Glycic acid	63	0.669	0.932	11.468	0.613	17	124	17	124	56	37 duplicate
4605	38	[708; 2,3-Dimethylsuccin	129	[840; Maltose methoxyamine (6TMS); alpha-D-Glc-(1,4)-D-Glc]	59	0.669	0.940	8.996	0.617	18	123	13	128	35	33 original
4538	38	[708; 2,3-Dimethylsuccin	62	[812; D-Xylofuranose (4TMS)]	64	0.669	0.893	8.366	0.645	19	122	23	118	29	19 original
4564	38	[708; 2,3-Dimethylsuccin	88	Gluconic acid	64	0.667	0.896	6.395	0.628	20	121	22	119	11	28 original
4516	38	[708; 2,3-Dimethylsuccin	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.660	0.891	29.741	0.612	21	120	24	117	132	38 original
4552	38	[708; 2,3-Dimethylsuccin	76	Fructose	64	0.656	0.857	19.899	0.608	22	119	28	113	106	40 original
4591	38	[708; 2,3-Dimethylsuccin	115	Glucose-6-phosphate	62	0.640	0.836	19.169	0.601	23	118	31	110	101	43 original
4554	38	[708; 2,3-Dimethylsuccin	78	Mannose	62	0.629	0.825	9.858	0.556	24	117	35	106	43	59 original
12689	38	[708; 2,3-Dimethylsuccin	22	[690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.623	0.945	12.331	0.625	25	116	10	131	64	30 duplicate
4582	38	[708; 2,3-Dimethylsuccin	106	[733; Threitol (4TMS)]	62	0.620	0.871	6.388	0.678	26	115	27	114	10	4 original
14145	38	[708; 2,3-Dimethylsuccin	35	Pyrogulonic acid	64	0.616	0.835	36.405	0.567	27	114	32	109	138	55 duplicate
4549	38	[708; 2,3-Dimethylsuccin	73	[708; Glucose methoxyamine (5TMS)]	57	0.614	0.775	8.956	0.489	28	113	41	100	34	79 original
4530	38	[708; 2,3-Dimethylsuccin	54	[NA]	55	0.609	0.889	12.057	0.630	29	112	25	116	61	27 original
12570	38	[708; 2,3-Dimethylsuccin	21	[678; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	64	0.581	0.820	11.040	0.585	30	111	37	104	52	50 duplicate
4579	38	[708; 2,3-Dimethylsuccin	103	[648; Ethylamine (2TMS)]	63	0.576	0.812	10.231	0.568	31	110	39	102	47	54 original
4568	38	[708; 2,3-Dimethylsuccin	92	[680; Glyceral-2-phosphate (4TMS)]	54	0.568	0.711	7.761	0.540	32	109	49	92	24	63 original
4546	38	[708; 2,3-Dimethylsuccin	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	0.559	0.580	13.832	0.439	33	108	61	80	70	105 original
4601	38	[708; 2,3-Dimethylsuccin	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	0.558	0.738	26.659	0.542	34	107	46	95	126	61 original
4576	38	[708; 2,3-Dimethylsuccin	100	[857; Mannitol (6TMS)]	64	0.552	0.840	3.201	0.557	35	106	30	111	4	58 original
13155	38	[708; 2,3-Dimethylsuccin	26	Citramalic acid	64	0.535	0.824	11.260	0.549	36	105	36	105	53	60 duplicate
4593	38	[708; 2,3-Dimethylsuccin	117	[724; Glyceral (3TMS)]	56	0.531	0.827	7.571	0.593	37	104	34	107	22	47 original
4598	38	[708; 2,3-Dimethylsuccin	121	[644; Erythritol (4TMS)]	52	0.529	0.875	16.094	0.613	38	103	26	115	81	36 original
4597	38	[708; 2,3-Dimethylsuccin	122	[657; Erythritol (4TMS)]	55	0.526	0.775	14.793	0.598	39	102	42	99	76	44 original

4586	38 [708; 2,3-Dimethylsuccr 110 [715; Erythritol (4TMS)]	54	0.522	0.833	11.368	0.643	40	101	33	108	55	21 original
4596	38 [708; 2,3-Dimethylsuccr 120 [945; Uridine (3TMS)]	54	0.494	0.359	7.135	0.651	41	100	71	70	18	17 original
4578	38 [708; 2,3-Dimethylsuccr 102 [904; Galactose methoxyamine (5TMS)]	64	0.492	0.756	6.611	0.558	42	99	44	97	16	57 original
4575	38 [708; 2,3-Dimethylsuccr 99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	0.488	0.933	11.475	0.655	43	98	16	125	57	16 original
4581	38 [708; 2,3-Dimethylsuccr 105 [705; 2-Ketogluconic acid (5TMS)]	48	0.484	0.820	8.490	0.604	44	97	38	103	31	42 original
4604	38 [708; 2,3-Dimethylsuccr 128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.483	0.850	4.733	0.625	45	96	29	112	8	31 original
4577	38 [708; 2,3-Dimethylsuccr 101 [832; Dopamine (4TMS)]	64	0.475	0.696	7.676	0.482	46	95	51	90	23	82 original
4598	38 [708; 2,3-Dimethylsuccr 112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.467	0.770	17.892	0.521	47	94	43	98	91	70 original
4520	38 [708; 2,3-Dimethylsuccr 44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	0.460	0.792	7.156	0.646	48	93	40	101	19	18 original
4569	38 [708; 2,3-Dimethylsuccr 113 Galactose-6-phosphate	62	0.457	0.718	8.489	0.524	49	92	47	94	30	69 original
10655	38 [708; 2,3-Dimethylsuccr 6 Glycerol	64	0.448	0.628	37.061	0.470	50	91	57	84	139	87 duplicate
4573	38 [708; 2,3-Dimethylsuccr 97 [756; beta-D-Methylglucopyranoside (4TMS)]	52	0.446	0.696	16.220	0.508	51	90	52	89	82	74 original
12207	38 [708; 2,3-Dimethylsuccr 18 [590; 1-Acetyl-2-thiohydantoin]	64	0.440	0.622	3.839	0.469	52	89	59	82	5	88 duplicate
4611	38 [708; 2,3-Dimethylsuccr 135	64	0.420	0.684	7.306	0.484	53	88	53	88	20	81 original
4561	38 [708; 2,3-Dimethylsuccr 85 [902; Melibiose (6TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	48	0.410	0.748	3.093	0.466	54	87	45	96	2	91 original
4602	38 [708; 2,3-Dimethylsuccr 126 [559; Erythritol (4TMS)]	45	0.408	0.677	9.004	0.661	55	86	54	87	36	15 original
4567	38 [708; 2,3-Dimethylsuccr 91 [766; beta-D-Methylglucopyranoside (4TMS)]	64	0.404	0.623	14.419	0.451	56	85	58	83	73	98 original
4590	38 [708; 2,3-Dimethylsuccr 114 Fructose-6-phosphate	53	0.382	0.704	9.444	0.535	57	84	50	91	41	64 original
4608	38 [708; 2,3-Dimethylsuccr 132 [895; Isomaltose methoxyamine (8TMS)]	42	0.377	0.940	16.047	0.638	58	83	12	129	80	24 original
4563	38 [708; 2,3-Dimethylsuccr 87 [945; beta-D-Glucopyranose (5TMS)]	62	0.354	0.634	30.329	0.458	59	82	56	85	135	96 original
4603	38 [708; 2,3-Dimethylsuccr 127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.352	0.711	5.902	0.665	60	81	48	93	9	11 original
4550	38 [708; 2,3-Dimethylsuccr 74 [912; Tetradeanoic acid (1TMS)]	64	0.348	0.649	9.055	0.499	61	80	55	86	37	78 original
12329	38 [708; 2,3-Dimethylsuccr 19 Alanine (BP) (3TMS)	64	0.325	0.587	7.088	0.458	62	79	60	81	17	97 duplicate
4592	38 [708; 2,3-Dimethylsuccr 116 [882; Pseudouridine (5TMS)]	30	0.310	0.486	8.618	0.377	63	78	84	77	32	133 original
4580	38 [708; 2,3-Dimethylsuccr 104 [795; Erythritol (4TMS)]	63	0.305	0.458	6.586	0.366	64	77	65	76	15	93 original
4559	38 [708; 2,3-Dimethylsuccr 83 Sorbitol	58	0.267	-0.268	18.114	0.368	65	76	92	49	93	135 original
4517	38 [708; 2,3-Dimethylsuccr 41 [639; Proline (2TMS)]	64	0.255	0.444	8.910	0.414	66	75	67	74	33	121 original
4599	38 [708; 2,3-Dimethylsuccr 123 [945; Galactofuranose-6-phosphate (7TMS)]	64	0.250	0.401	6.416	0.465	67	74	70	71	13	92 original
4572	38 [708; 2,3-Dimethylsuccr 96 myo-Inositol	49	0.218	0.235	20.115	0.292	68	73	76	65	108	140 original
4556	38 [708; 2,3-Dimethylsuccr 80 [772; D-Glucose (5TMS)]	62	0.205	0.506	25.978	0.415	69	72	62	79	122	120 original
9980	38 [708; 2,3-Dimethylsuccr 1 [938; Sulfuric acid (2TMS)]	36	0.187	0.438	9.345	0.614	70	71	68	73	40	35 duplicate
4560	38 [708; 2,3-Dimethylsuccr 84 Mannitol	62	0.182	0.500	26.963	0.461	71	70	63	78	127	94 original
4540	38 [708; 2,3-Dimethylsuccr 64 [789; Tyramine (3TMS)]	63	0.181	0.208	6.414	0.451	72	69	78	63	12	99 original
11835	38 [708; 2,3-Dimethylsuccr 15 Alanine	42	0.150	0.341	21.796	0.429	73	68	72	69	114	114 original
4555	38 [708; 2,3-Dimethylsuccr 78 Glucose	64	0.146	0.216	14.191	0.595	74	67	77	64	72	45 duplicate
4609	38 [708; 2,3-Dimethylsuccr 133 [855; Squalene]	64	0.131	0.447	30.191	0.533	75	66	66	75	133	65 original
4569	38 [708; 2,3-Dimethylsuccr 93 [607; Putrescine (4TMS)]	64	0.129	0.042	7.815	0.376	76	65	83	58	25	134 original
4585	38 [708; 2,3-Dimethylsuccr 109 Octadecanoic acid	64	0.091	0.432	18.004	0.486	78	63	69	72	92	80 original
4616	38 [708; 2,3-Dimethylsuccr 140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49	0.071	0.244	16.601	0.417	79	62	75	66	83	118 original
4523	38 [708; 2,3-Dimethylsuccr 47 [NA]	64	0.065	0.100	10.908	0.444	80	61	80	61	51	102 original
4570	38 [708; 2,3-Dimethylsuccr 94 Hexadecanoic acid	64	0.033	0.341	17.083	0.477	81	60	73	68	85	84 original
4617	38 [708; 2,3-Dimethylsuccr 141 Lanosta-8,24-dien-3-beta-ol	61	0.021	0.167	15.054	0.440	82	59	79	62	77	104 original
4614	38 [708; 2,3-Dimethylsuccr 138 [674; Ergosterol (1TMS)]	46	0.014	0.084	17.756	0.430	83	58	82	59	89	112 original
4528	38 [708; 2,3-Dimethylsuccr 53 Glycerol-2-phosphate	64	-0.024	-0.104	12.616	0.329	84	57	87	54	65	138 original
4594	38 [708; 2,3-Dimethylsuccr 118 [928; Glucopyranose-6-phosphate (6TMS)]	58	-0.028	0.084	10.590	0.399	85	56	81	60	49	128 original
4547	38 [708; 2,3-Dimethylsuccr 71 [731; Erythrose (3TMS)]	64	-0.041	-0.126	8.149	0.427	86	55	88	53	27	117 original
4613	38 [708; 2,3-Dimethylsuccr 137 Ergosterol	64	-0.057	-0.092	12.179	0.427	87	54	86	55	62	116 original
4568	38 [708; 2,3-Dimethylsuccr 90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	64	-0.060	-0.021	6.556	0.411	88	53	84	57	14	123 original
4615	38 [708; 2,3-Dimethylsuccr 139 [930; Ergosta-5,7-dien-3-ol]	38	-0.084	-0.155	19.509	0.380	89	52	89	52	103	131 original

4595	38 [708; 2,3-Dimethylsucr	119 [931; myo-Inositol-2-phosphate (7TMS)]	64 -0,109	-0,037	7,921	0,428	90	51	85	56	26	115 original
4593	38 [708; 2,3-Dimethylsucr	107 9-(Z)-Octadecenoic acid	64 -0,145	-0,234	10,806	0,402	91	50	91	50	50	125 original
4539	38 [708; 2,3-Dimethylsucr	63 Glutamine	52 -0,154	-0,665	19,074	0,627	92	49	116	25	100	29 original
	124 [734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecenoyleglycerol (1TMS)]											
4600	38 [708; 2,3-Dimethylsucr	72 [819; D-Xylopyranose (4TMS)]	59 -0,162	-0,304	25,286	0,430	83	48	93	48	120	113 original
4548	38 [708; 2,3-Dimethylsucr	68 [570; Hypoxanthine (2TMS)]	63 -0,163	-0,231	11,332	0,345	84	47	90	51	54	137 original
4544	38 [708; 2,3-Dimethylsucr	4 Phosphoric acid	20 -0,211	-0,892	15,174	0,508	95	46	135	6	78	75 original
10394	38 [708; 2,3-Dimethylsucr	130 Trehalose	51 -0,224	-0,428	30,267	0,302	96	45	97	44	134	139 duplicate
4606	38 [708; 2,3-Dimethylsucr	7 Threonine	53 -0,227	-0,413	25,561	0,391	97	44	96	45	121	130 original
10799	38 [708; 2,3-Dimethylsucr	43 [548; Leucine (2TBS)]	64 -0,255	-0,517	26,043	0,416	98	43	102	39	123	119 duplicate
4519	38 [708; 2,3-Dimethylsucr	52 [NA]	60 -0,255	-0,491	8,318	0,435	99	42	99	42	28	110 original
4528	38 [708; 2,3-Dimethylsucr	36 [596; N-Acetylglutamic acid (2TMS)]	46 -0,262	-0,579	21,903	0,587	100	41	107	34	115	49 original
14250	38 [708; 2,3-Dimethylsucr	66 Glyceric acid-3-phosphate	64 -0,275	-0,544	25,109	0,436	101	40	105	36	119	109 duplicate
4542	38 [708; 2,3-Dimethylsucr	58 [636; 4R-Acetamidido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64 -0,286	-0,618	9,250	0,531	102	39	110	31	38	66 original
4534	38 [708; 2,3-Dimethylsucr	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	64 -0,287	-0,479	13,889	0,394	103	38	98	43	71	128 original
4612	38 [708; 2,3-Dimethylsucr	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	17 -0,294	-0,329	4,608	0,468	104	37	94	47	7	89 original
13268	38 [708; 2,3-Dimethylsucr	98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	53 -0,296	-0,865	21,558	0,582	105	36	134	7	113	51 duplicate
4574	38 [708; 2,3-Dimethylsucr	61 [NA]	48 -0,298	-0,826	20,797	0,559	106	35	130	11	112	56 original
4537	38 [708; 2,3-Dimethylsucr	75 Lysine	64 -0,302	-0,368	7,343	0,459	107	34	95	46	21	95 original
4551	38 [708; 2,3-Dimethylsucr	2 Serine	64 -0,313	-0,571	35,741	0,413	108	33	106	35	137	122 original
10119	38 [708; 2,3-Dimethylsucr	8 Isoleucine	62 -0,319	-0,616	18,902	0,437	109	32	109	32	99	108 duplicate
10832	38 [708; 2,3-Dimethylsucr	108 Octadecenoic acid	55 -0,329	-0,534	18,185	0,345	110	31	104	37	94	136 duplicate
4594	38 [708; 2,3-Dimethylsucr	25 [709; 2,5-Diaminovalerolactam (2TMS)]	64 -0,336	-0,495	10,111	0,380	111	30	100	41	45	132 original
13040	38 [708; 2,3-Dimethylsucr	67 Citric acid	48 -0,342	-0,930	18,880	0,638	112	29	139	2	98	23 duplicate
4543	38 [708; 2,3-Dimethylsucr	37 Phenylalanine	64 -0,363	-0,527	19,557	0,410	113	28	103	38	104	124 original
14354	38 [708; 2,3-Dimethylsucr	23 Homoserine	64 -0,364	-0,623	18,766	0,446	114	26	112	29	97	101 duplicate
12807	38 [708; 2,3-Dimethylsucr	30 Glycerol-3-phosphate	64 -0,364	-0,892	13,601	0,618	115	27	136	5	68	32 duplicate
4536	38 [708; 2,3-Dimethylsucr	61 [622; Parabenic acid (2TMS)]	64 -0,367	-0,505	17,671	0,437	116	25	101	40	87	106 original
13715	38 [708; 2,3-Dimethylsucr	89 [775; Dopamine (4TMS)]	64 -0,383	-0,728	13,710	0,540	117	24	119	22	69	62 duplicate
4565	38 [708; 2,3-Dimethylsucr	9 Proline	3									

4558	38 [708; 2,3-Dimethylsuccin	82	Lysine	39	-0.646	-0.931	17,757	0.588	138	3	140	1	90	48 original
4518	38 [708; 2,3-Dimethylsuccin	42	Glutamic acid	60	-0.647	-0.812	28,727	0.501	139	2	127	14	130	77 original
12450	38 [708; 2,3-Dimethylsuccin													
11961	39 [829; 1-Phenylethanol (1	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	31	-0.716	-0.843	15,230	0.573	140	1	131	10	79	53 duplicate
12925	39 [829; 1-Phenylethanol (1	24	[725; 2-Ketooctanoic acid (2TMS)]	63	0.823	0.980	8,659	0.988	1	140	2	139	6	3 duplicate
11583	39 [829; 1-Phenylethanol (1	13	Uracil	63	0.814	0.980	20,865	0.981	2	139	1	140	83	6 duplicate
4634	39 [829; 1-Phenylethanol (1	56	[829; Oxalic acid (3TMS)]	63	0.804	0.979	5,338	0.988	3	138	3	138	2	4 duplicate
4624	39 [829; 1-Phenylethanol (1	49	Arabinose	63	0.795	0.957	13,013	0.978	4	137	8	133	36	8 original
13495	39 [829; 1-Phenylethanol (1	28	Erythritol	63	0.790	0.951	4,898	0.977	5	136	11	130	1	9 original
4664	39 [829; 1-Phenylethanol (1	96	[793; D-Galactono-1,4-lactone (4TMS)]	63	0.789	0.962	14,074	0.960	6	135	7	134	42	14 duplicate
4707	39 [829; 1-Phenylethanol (1	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	60	0.784	0.925	9,087	0.975	7	134	18	123	8	10 original
4843	39 [829; 1-Phenylethanol (1	65	[646; 3-Deoxyglucitol (5TMS)]	59	0.771	0.966	10,681	0.932	8	133	9	132	18	22 original
	39 [829; 1-Phenylethanol (1	57		63	0.765	0.969	12,632	0.700	9	132	5	136	34	1 original
4635	39 [829; 1-Phenylethanol (1		[757; 2-Deoxy-pentose-3-yose dimethoxyamine (2TMS)]	55	0.762	0.933	8,133	0.651	10	131	15	126	4	18 original
12085	39 [829; 1-Phenylethanol (1	134	Isomaltose	63	0.755	0.987	11,019	0.693	11	130	6	135	22	2 original
4628	39 [829; 1-Phenylethanol (1	17	[700; 2-methyl-1,2-propanediol (2TMS)]	63	0.748	0.916	8,150	0.603	12	129	19	122	5	45 duplicate
14458	39 [829; 1-Phenylethanol (1	50	[746; Ribonic acid-1,4-lactone (3TMS)]	60	0.736	0.953	26,750	0.626	13	128	10	131	118	23 original
4668	39 [829; 1-Phenylethanol (1	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	63	0.714	0.972	10,377	0.666	14	127	4	137	13	13 duplicate
4640	39 [829; 1-Phenylethanol (1	88	Gluconic acid	63	0.701	0.905	6,700	0.636	15	126	21	120	3	20 original
11328	39 [829; 1-Phenylethanol (1	62	[812; D-Xylofuranose (4TMS)]	63	0.697	0.895	9,891	0.621	16	125	23	118	12	28 original
4632	39 [829; 1-Phenylethanol (1	11	Succinic acid	63	0.685	0.887	11,284	0.612	17	124	22	119	25	38 duplicate
4677	39 [829; 1-Phenylethanol (1	54	[NA]	54	0.684	0.891	18,130	0.572	18	123	24	117	68	52 original
11710	39 [829; 1-Phenylethanol (1	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	0.673	0.933	18,939	0.660	19	122	14	127	78	15 original
12690	39 [829; 1-Phenylethanol (1	14	Fumaric acid	63	0.653	0.939	17,925	0.687	20	121	12	129	67	12 duplicate
11455	39 [829; 1-Phenylethanol (1	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.637	0.929	18,668	0.619	21	120	16	125	71	29 duplicate
13383	39 [829; 1-Phenylethanol (1	12	Glyceric acid	62	0.627	0.909	19,700	0.613	22	119	20	121	80	36 duplicate
4684	39 [829; 1-Phenylethanol (1	28	Malic acid	63	0.620	0.937	10,475	0.680	23	118	13	128	15	7 duplicate
4651	39 [829; 1-Phenylethanol (1	106	[733; Threitol (4TMS)]	61	0.616	0.877	8,732	0.667	24	117	25	116	7	11 original
4656	39 [829; 1-Phenylethanol (1	73	[708; Glucose methoxyamine (5TMS)]	56	0.610	0.774	12,611	0.490	25	116	42	99	33	78 original
4654	39 [829; 1-Phenylethanol (1	78	Mannose	61	0.610	0.833	14,781	0.571	26	115	32	108	48	53 original
4681	39 [829; 1-Phenylethanol (1	76	Fructose	63	0.605	0.857	13,947	0.616	27	114	28	113	40	33 original
4863	39 [829; 1-Phenylethanol (1	103	[648; Ethylamine (2TMS)]	62	0.601	0.821	9,202	0.541	28	113	35	106	9	62 original
4618	39 [829; 1-Phenylethanol (1	105	[705; 2-Ketogluconic acid (5TMS)]	48	0.594	0.853	9,690	0.568	29	112	29	112	11	56 original
4670	39 [829; 1-Phenylethanol (1	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	63	0.583	0.861	25,800	0.611	30	111	27	114	111	39 original
4648	39 [829; 1-Phenylethanol (1	92	[680; Glycerol-2-phosphate (4TMS)]	53	0.582	0.713	13,646	0.532	31	110	46	95	38	66 original
4695	39 [829; 1-Phenylethanol (1	117	[724; Glycerol (3TMS)]	56	0.560	0.576	12,347	0.488	32	109	59	82	31	79 original
4703	39 [829; 1-Phenylethanol (1	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	63	0.553	0.838	13,810	0.602	33	108	31	110	39	46 original
4693	39 [829; 1-Phenylethanol (1	115	Glucose-6-phosphate	63	0.545	0.736	21,174	0.563	34	107	44	97	84	57 original
14146	39 [829; 1-Phenylethanol (1	35	Pyroglutamic acid	61	0.541	0.821	14,624	0.603	35	106	36	105	47	44 original
12571	39 [829; 1-Phenylethanol (1	21	[676; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	63	0.538	0.828	31,364	0.604	36	104	33	108	134	43 duplicate
4675	39 [829; 1-Phenylethanol (1	97	[756; beta-D-Methylglucopyranoside (4TMS)]	63	0.538	0.778	10,976	0.570	37	103	40	101	21	55 duplicate
4688	39 [829; 1-Phenylethanol (1	110	[715; Erythritol (4TMS)]	52	0.534	0.738	10,660	0.483	38	103	43	98	17	83 original
4679	39 [829; 1-Phenylethanol (1	26	Citramalic acid	54	0.523	0.843	16,398	0.655	39	102	30	111	59	17 original
4699	39 [829; 1-Phenylethanol (1	101	[832; Dopamine (4TMS)]	63	0.512	0.789	12,343	0.551	40	101	38	103	30	61 duplicate
4700	39 [829; 1-Phenylethanol (1	121	[657; Erythritol (4TMS)]	63	0.508	0.707	11,368	0.482	41	100	49	92	26	86 original
4698	39 [829; 1-Phenylethanol (1	122	[644; Erythritol (4TMS)]	54	0.501	0.777	22,159	0.613	42	99	41	100	92	35 original
4698	39 [829; 1-Phenylethanol (1	120	[945; Uridine (3TMS)]	52	0.486	0.876	22,346	0.608	43	98	26	115	83	41 original
4678	39 [829; 1-Phenylethanol (1	100	[857; Mannitol (6TMS)]	54	0.480	0.363	10,932	0.642	44	97	71	70	20	19 original
	39 [829; 1-Phenylethanol (1			63	0.471	0.797	11,123	0.551	45	95	39	102	24	60 original

4669	39 [829; 1-Phenylethanol (1 91 [766; beta-D-Methylglucopyranoside (4TMS)]	63	0.471	0.855	14.004	0.435	48	96	54	87	41	111 original
4706	39 [829; 1-Phenylethanol (1 128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.465	0.826	10.465	0.578	47	94	34	107	14	51 original
10668	39 [829; 1-Phenylethanol (1 6 Glyceral	63	0.464	0.653	32.278	0.480	49	93	55	86	136	88 duplicate
4622	39 [829; 1-Phenylethanol (1 44 [910; 2-Ketogluconic acid methoxymine (4TMS)]	50	0.461	0.809	11.074	0.593	48	92	37	104	23	47 original
4665	39 [829; 1-Phenylethanol (1 87 [945; beta-D-Glucopyranose (5TMS)]	61	0.431	0.658	25.000	0.477	50	91	53	88	107	90 original
4680	39 [829; 1-Phenylethanol (1 102 [904; Galactose methoxymine (5TMS)]	63	0.428	0.709	16.139	0.534	51	90	48	93	54	65 original
4690	39 [829; 1-Phenylethanol (1 112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	62	0.420	0.692	26.307	0.516	52	89	50	91	113	70 original
9981	39 [829; 1-Phenylethanol (1 1 [938; Sulfuric acid (2TMS)]	36	0.413	0.558	16.923	0.589	53	88	61	80	62	48 duplicate
4663	39 [829; 1-Phenylethanol (1 85 [529; Methylenic acid (4TMS)]	47	0.395	0.731	9.639	0.456	54	87	45	96	10	97 original
135												
4713	39 [829; 1-Phenylethanol (1 [902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	63	0.370	0.614	12.009	0.478	55	86	58	83	28	89 original
12208	39 [829; 1-Phenylethanol (1 18 [590; 1-Acetyl-2-hydroxydantoin]	63	0.354	0.545	12.716	0.453	56	85	62	79	35	99 duplicate
4691	39 [829; 1-Phenylethanol (1 113 Galactose-6-phosphate	61	0.349	0.683	15.924	0.495	57	84	52	89	52	74 original
4652	39 [829; 1-Phenylethanol (1 74 [912; Tetradecanoic acid (1TMS)]	63	0.310	0.624	15.073	0.484	58	83	57	84	49	81 original
4682	39 [829; 1-Phenylethanol (1 104 [795; Erythritol (4TMS)]	62	0.309	0.470	14.074	0.473	59	82	65	78	43	93 original
12330	39 [829; 1-Phenylethanol (1 19 Alanine (BP) (3TMS)	63	0.303	0.572	10.736	0.482	60	81	60	81	19	85 duplicate
4705	39 [829; 1-Phenylethanol (1 127 [777; Fructose-6-phosphate methoxymine (6TMS)]	39	0.287	0.709	14.432	0.634	61	80	47	94	45	21 original
4710	39 [829; 1-Phenylethanol (1 132 [895; Isomaltose methoxymine (8TMS)]	42	0.282	0.927	21.627	0.626	62	79	17	124	87	24 original
4704	39 [829; 1-Phenylethanol (1 114 Fructose-6-phosphate	45	0.277	0.642	16.867	0.612	63	78	56	85	61	37 original
4692	39 [829; 1-Phenylethanol (1 80 [772; D-Glucose (5TMS)]	52	0.256	0.894	17.324	0.559	64	77	51	90	65	59 original
4658	39 [829; 1-Phenylethanol (1 116 [882; Pseudouridine (5TMS)]	61	0.251	0.527	21.579	0.435	65	76	63	78	86	110 original
4684	39 [829; 1-Phenylethanol (1 84 Mannitol	30	0.223	0.430	12.501	0.417	66	75	67	74	32	121 original
4662	39 [829; 1-Phenylethanol (1 84 Mannitol	61	0.217	0.505	22.581	0.448	67	74	64	77	95	102 original
4619	39 [829; 1-Phenylethanol (1 41 [639; Proline (2TMS)]	63	0.196	0.416	11.794	0.443	68	73	68	73	27	108 original
4674	39 [829; 1-Phenylethanol (1 96 myo-Inositol	48	0.179	0.220	26.613	0.326	69	72	76	65	116	139 original
4701	39 [829; 1-Phenylethanol (1 123 [945; Galactofuranose-6-phosphate (7TMS)]	63	0.172	0.387	12.112	0.494	70	71	70	71	29	82 original
4671	39 [829; 1-Phenylethanol (1 93 [607; Putrescine (4TMS)]	60	0.168	0.339	25.094	0.375	71	70	72	69	108	132 original
4625	39 [829; 1-Phenylethanol (1 47 [NA]	63	0.164	0.156	17.316	0.444	72	69	80	61	84	108 original
4661	39 [829; 1-Phenylethanol (1 83 Sorbitol	57	0.145	-0.293	19.182	0.358	73	68	93	48	77	135 original
4642	39 [829; 1-Phenylethanol (1 64 [789; Tyramine (3TMS)]	62	0.111	0.180	16.340	0.389	74	67	78	63	57	129 original
11836	39 [829; 1-Phenylethanol (1 15 Alanine	63	0.091	0.214	14.542	0.624	75	66	77	64	46	26 duplicate
4657	39 [829; 1-Phenylethanol (1 79 Glucose	63	0.078	0.446	25.879	0.532	76	65	66	75	112	67 original
4631	39 [829; 1-Phenylethanol (1 53 Glycerol-2-phosphate	63	0.040	-0.033	21.836	0.356	77	64	85	56	88	136 original
4689	39 [829; 1-Phenylethanol (1 111 [583; Erythritol (4TMS)]	41	0.039	0.288	29.976	0.417	78	63	74	67	131	120 original
4718	39 [829; 1-Phenylethanol (1 140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	48	0.037	0.279	23.527	0.446	79	62	75	66	99	103 original
4687	39 [829; 1-Phenylethanol (1 109 Octadecanoic acid	63	0.035	0.397	16.021	0.477	80	61	69	72	53	91 original
4711	39 [829; 1-Phenylethanol (1 133 [855; Squalene]	63	0.018	0.001	16.339	0.362	81	60	84	57	56	133 original
4668	39 [829; 1-Phenylethanol (1 90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	63	0.012	0.052	15.105	0.377	82	59	82	59	50	131 original
4672	39 [829; 1-Phenylethanol (1 94 Hexadecanoic acid	63	-0.027	0.313	15.650	0.468	83	58	73	68	51	95 original
4719	39 [829; 1-Phenylethanol (1 141 Lanosta-8,24-dien-3-beta-ol	60	-0.047	0.165	22.915	0.449	84	57	79	62	96	101 original
4696	39 [829; 1-Phenylethanol (1 118 [928; Glucopyranose-6-phosphate (6TMS)]	58	-0.060	0.098	18.937	0.400	85	56	81	60	75	127 original
4641	39 [829; 1-Phenylethanol (1 63 Glutamine	51	-0.100	-0.721	28.274	0.687	86	55	118	23	124	5 original
4650	39 [829; 1-Phenylethanol (1 138 [674; Ergosterol (1TMS)]	46	-0.125	0.042	25.674	0.445	87	54	83	58	110	104 original
4716	39 [829; 1-Phenylethanol (1 72 [919; D-Xylopyranose (4TMS)]	62	-0.126	-0.221	20.118	0.317	88	53	91	50	82	140 original
4685	39 [829; 1-Phenylethanol (1 107 9-(Z)-Octadecenoic acid	63	-0.132	-0.193	14.151	0.390	89	52	89	52	44	128 original
4715	39 [829; 1-Phenylethanol (1 137 Ergosterol	63	-0.137	-0.114	16.668	0.427	90	51	87	54	60	114 original
4697	39 [829; 1-Phenylethanol (1 119 [931; myo-Inositol-2-phosphate (7TMS)]	63	-0.156	-0.043	16.149	0.445	91	49	86	55	55	105 original
4649	39 [829; 1-Phenylethanol (1 71 [731; Erythrose (3TMS)]	63	-0.166	-0.203	13.539	0.419	92	50	90	51	37	119 original
4630	39 [829; 1-Phenylethanol (1 52 [NA]	45	-0.158	-0.549	29.856	0.618	93	48	101	40	130	32 original
10395	39 [829; 1-Phenylethanol (1 4 Phosphoric acid	50	-0.207	-0.427	28.658	0.331	94	47	96	45	125	138 duplicate
4717	39 [829; 1-Phenylethanol (1 139 [700; Ergosta-5,7-dien-3-ol]	37	-0.219	-0.142	26.612	0.431	95	46	88	53	115	112 original

4708	39 [829; 1-Phenylethanol (1 130 Trehalose	62 -0.219	-0.363	23.003	0.402	96	45	94	47	97	124 original
	124 [734; 1-Monooleoylglycerol (2TMS); 1-										
4702	39 [829; 1-Phenylethanol (1 124	58 -0.232	-0.289	33.435	0.422	97	44	92	49	139	117 original
4621	39 [829; 1-Phenylethanol (1 43 [548; Leucine (2TMS)]	59 -0.233	-0.458	16.380	0.468	98	43	97	44	58	94 original
4646	39 [829; 1-Phenylethanol (1 68 [570; Hypoxanthine (2TMS)]	20 -0.242	-0.908	19.283	0.583	99	42	136	5	78	50 original
13041	39 [829; 1-Phenylethanol (1 25 [709; 2,5-Diaminovalerolactam (2TMS)]	48 -0.261	-0.913	28.131	0.623	100	41	137	4	122	27 duplicate
4638	39 [829; 1-Phenylethanol (1 58 [636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane										
	(1TMS)]										
4639	39 [829; 1-Phenylethanol (1 61 [NA]	63 -0.290	-0.461	17.809	0.380	101	40	98	43	66	130 original
4686	39 [829; 1-Phenylethanol (1 108 Octadecenoic acid	63 -0.294	-0.405	17.097	0.454	102	39	95	46	63	98 original
4676	39 [829; 1-Phenylethanol (1 98 [697; Ribose-5-phosphate methoxamine (5TMS)]	47 -0.321	-0.823	28.207	0.560	103	38	99	42	81	123 original
14251	39 [829; 1-Phenylethanol (1 36 [596; N-Acetylglutamic acid (2TMS)]	63 -0.329	-0.574	24.238	0.424	105	36	106	35	104	115 duplicate
4653	39 [829; 1-Phenylethanol (1 75 Lysine	63 -0.335	-0.565	32.635	0.416	106	35	103	38	138	122 original
12808	39 [829; 1-Phenylethanol (1 23 Homoserine	63 -0.339	-0.865	22.442	0.618	107	34	134	7	94	31 duplicate
10800	39 [829; 1-Phenylethanol (1 7 Threonine	63 -0.364	-0.558	23.984	0.401	108	33	102	39	101	125 duplicate
13270	39 [829; 1-Phenylethanol (1 27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	52 -0.373	-0.860	29.499	0.571	109	32	132	9	128	54 duplicate
4644	39 [829; 1-Phenylethanol (1 66 Glycetic acid-3-phosphate	63 -0.398	-0.664	19.335	0.486	110	31	112	29	79	80 original
4667	39 [829; 1-Phenylethanol (1 89 [775; Dopamine (4TMS)]	34 -0.401	-0.789	24.608	0.537	111	30	124	17	106	64 original
4709	39 [829; 1-Phenylethanol (1 131 [628; 5-Methylthioadenosine (3TMS)]	54 -0.412	-0.670	26.465	0.511	112	29	113	28	114	71 original
4623	39 [829; 1-Phenylethanol (1 45 Homocysteine	60 -0.423	-0.630	31.806	0.444	113	28	110	31	135	107 original
4626	39 [829; 1-Phenylethanol (1 48 Asparagine	63 -0.432	-0.810	23.489	0.610	114	27	125	16	98	40 original
4638	39 [829; 1-Phenylethanol (1 60 Glycerol-3-phosphate	63 -0.436	-0.566	18.346	0.451	115	26	104	37	70	100 original
4627	39 [829; 1-Phenylethanol (1 49 [877; Pyrophosphoric acid (4TMS)]	63 -0.437	-0.592	32.372	0.477	116	25	108	33	137	92 original
4645	39 [829; 1-Phenylethanol (1 67 Citric acid	63 -0.439	-0.578	18.746	0.361	117	24	107	34	74	134 original
4714	39 [829; 1-Phenylethanol (1 136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17 -0.441	-0.512	10.645	0.495	118	23	100	41	16	75 original
13716	39 [829; 1-Phenylethanol (1 31 [622; Parabanic acid (2TMS)]	63 -0.452	-0.734	23.558	0.541	119	22	119	22	100	63 duplicate
10120	39 [829; 1-Phenylethanol (1 2 Serine	61 -0.454	-0.850	24.083	0.424	120	21	111	30	102	116 duplicate
10933	39 [829; 1-Phenylethanol (1 8 Isoleucine	54 -0.458	-0.572	22.074	0.337	121	20	105	36	81	137 duplicate
4673	39 [829; 1-Phenylethanol (1 95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	49 -0.507	-0.625	27.512	0.400	122	19	109	32	119	126 original
14355	39 [829; 1-Phenylethanol (1 37 Phenylalanine	63 -0.508	-0.698	18.734	0.444	123	18	116	25	73	108 duplicate
4629	39 [829; 1-Phenylethanol (1 51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	43 -0.522	-0.827	25.482	0.482	124	17	128	13	109	87 original
14040	39 [829; 1-Phenylethanol (1 34 Aspartic acid	63 -0.524	-0.672	28.062	0.486	125	16	114	27	121	73 duplicate
11065	39 [829; 1-Phenylethanol (1 9 Proline	62 -0.525	-0.683	28.781	0.421	126	15	115	26	126	118 duplicate
4633	39 [829; 1-Phenylethanol (1 55 [612; 4-Aminobutyric acid (2TBS)]	42 -0.549	-0.715	26.748	0.462	127	14	117	24	117	96 original
13933	39 [829; 1-Phenylethanol (1 33 Methionine	63 -0.571	-0.748	22.044	0.509	128	13	122	19	90	72 duplicate
10258	39 [829; 1-Phenylethanol (1 3 Ethanolamine	61 -0.580	-0.787	24.135	0.517	129	12	123	18	103	69 duplicate
	39 [829; 1-Phenylethanol (1										
12451	20 [619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	30 -0.586	-0.852	18.190	0.605	130	11	130	11	69	42 duplicate
13606	39 [829; 1-Phenylethanol (1 30 [615; Ethyl-3(2H)-thiophenone]	63 -0.606	-0.744	27.696	0.429	131	10	121	20	120	113 duplicate
10531	39 [829; 1-Phenylethanol (1 5 Leucine	44 -0.607	-0.860	18.699	0.524	132	9	133	8	72	68 duplicate
4637	39 [829; 1-Phenylethanol (1 59 Ornithine; Arginine	63 -0.617	-0.736	34.206	0.490	133	8	120	21	140	77 original
11196	39 [829; 1-Phenylethanol (1 10 Glycine	63 -0.623	-0.933	21.260	0.659	134	7	139	2	85	16 duplicate
4647	39 [829; 1-Phenylethanol (1 69 Arginine	59 -0.643	-0.922	24.497	0.619	135	6	138	3	105	30 original
13825	39 [829; 1-Phenylethanol (1 32 [729; N,N-Dimethyllysine methyl ester]	62 -0.650	-0.878	29.793	0.614	136	5	135	6	129	34 duplicate
	[726; beta-[[[5-methyl-2-thienyl)methyl]amino-										
	benzenecarboxylic acid methyl ester]										
4655	39 [829; 1-Phenylethanol (1 81 Tyrosine	61 -0.660	-0.811	29.287	0.491	137	4	126	15	127	76 original
4659	39 [829; 1-Phenylethanol (1 81 Tyrosine	63 -0.669	-0.859	30.971	0.584	138	3	131	10	132	49 original
4660	39 [829; 1-Phenylethanol (1 82 Lysine	38 -0.693	-0.936	21.971	0.624	139	2	140	1	89	25 original
4620	39 [829; 1-Phenylethanol (1 42 Glutamic acid	59 -0.719	-0.836	30.995	0.483	140	1	129	12	133	84 original
4755	40 [680; 2,3-Dimethylsuccin 76 Fructose	84 0.790	0.858	15.134	0.592	1	140	11	130	22	33 original
4785	40 [680; 2,3-Dimethylsuccin 106 [733; Threitol (4TMS)]	62 0.759	0.926	30.151	0.583	2	139	1	140	72	1 original



4801	40 [680; 2,3-Dimethylsuccin	122	[644; Erythritol (4TMS)]	52	0.730	0.904	41,124	0.816	3	138	3	138	119	14 original
4800	40 [680; 2,3-Dimethylsuccin	121	[657; Erythritol (4TMS)]	55	0.725	0.895	41,281	0.817	4	137	4	137	120	12 original
4723	40 [680; 2,3-Dimethylsuccin	44	[910; 2-Ketoglucuronic acid methoxyamine (4TMS)]	50	0.722	0.890	27,985	0.598	5	136	5	136	65	37 original
4789	40 [680; 2,3-Dimethylsuccin	110	[715; Erythritol (4TMS)]	54	0.712	0.876	35,791	0.639	6	135	6	135	102	5 original
13384	40 [680; 2,3-Dimethylsuccin	28	Malic acid	64	0.706	0.910	27,109	0.845	7	134	2	139	59	4 duplicate
4796	40 [680; 2,3-Dimethylsuccin	117	[724; Glycerol (3TMS)]	56	0.701	0.894	33,167	0.598	8	133	7	134	88	38 original
4794	40 [680; 2,3-Dimethylsuccin	126	[559; Erythritol (4TMS)]	62	0.695	0.827	11,802	0.599	9	132	24	117	15	34 original
4805	40 [680; 2,3-Dimethylsuccin	115	Glucose-6-phosphate	45	0.673	0.822	31,194	0.598	10	131	26	115	77	35 original
14147	40 [680; 2,3-Dimethylsuccin	35	Pyroglutamic acid	64	0.663	0.808	7,692	0.575	11	130	31	110	6	41 duplicate
14459	40 [680; 2,3-Dimethylsuccin	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.660	0.891	29,741	0.612	12	129	5	138	71	20 duplicate
4757	40 [680; 2,3-Dimethylsuccin	78	Mannose	62	0.657	0.835	37,274	0.582	13	128	22	119	107	40 original
4765	40 [680; 2,3-Dimethylsuccin	86	[793; D-Galactono-1,4-lactone (4TMS)]	61	0.650	0.852	27,196	0.630	14	127	14	127	60	8 original
11711	40 [680; 2,3-Dimethylsuccin	14	Fumaric acid	64	0.649	0.875	38,730	0.617	15	126	9	132	114	11 duplicate
12691	40 [680; 2,3-Dimethylsuccin	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.626	0.850	38,664	0.602	16	125	15	128	113	24 duplicate
4752	40 [680; 2,3-Dimethylsuccin	73	[708; Glucose methoxyamine (5TMS)]	57	0.617	0.839	35,039	0.567	17	124	19	122	97	46 original
13498	40 [680; 2,3-Dimethylsuccin	29	Erythritol	64	0.612	0.849	33,332	0.609	18	123	16	125	89	22 duplicate
4779	40 [680; 2,3-Dimethylsuccin	100	[857; Mannitol (6TMS)]	64	0.608	0.783	27,838	0.525	19	122	36	105	61	70 original
12926	40 [680; 2,3-Dimethylsuccin	24	[725; 2-Ketocanic acid (2TMS)]	64	0.605	0.858	7,259	0.615	20	120	12	129	4	15 duplicate
11327	40 [680; 2,3-Dimethylsuccin	11	Succinic acid	64	0.605	0.835	29,248	0.613	21	121	21	120	68	19 duplicate
4741	40 [680; 2,3-Dimethylsuccin	62	[812; D-Xylofuranose (4TMS)]	64	0.605	0.835	29,248	0.613	21	121	21	120	68	19 duplicate
12572	40 [680; 2,3-Dimethylsuccin	21	[878; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	0.604	0.815	21,643	0.597	22	119	27	114	41	28 original
11862	40 [680; 2,3-Dimethylsuccin	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	0.590	0.805	19,105	0.540	23	118	32	109	32	58 duplicate
14561	40 [680; 2,3-Dimethylsuccin	39	[829; 1-Phenylethanol (1TMS)]	64	0.585	0.845	18,700	0.614	24	117	18	123	29	17 duplicate
4725	40 [680; 2,3-Dimethylsuccin	46	Arabinose	63	0.583	0.861	25,800	0.611	25	116	10	131	55	21 duplicate
13157	40 [680; 2,3-Dimethylsuccin	26	Citramalic acid	64	0.578	0.831	27,881	0.633	26	115	23	118	63	6 original
4804	40 [680; 2,3-Dimethylsuccin	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	0.573	0.813	18,680	0.528	27	114	28	113	30	69 duplicate
4781	40 [680; 2,3-Dimethylsuccin	102	[904; Galactose methoxyamine (5TMS)]	64	0.570	0.710	10,935	0.530	28	113	45	98	12	66 original
4744	40 [680; 2,3-Dimethylsuccin	65	[646; 3-Deoxyglucitol (5TMS)]	64	0.566	0.736	35,444	0.515	29	112	43	98	99	76 original
4813	40 [680; 2,3-Dimethylsuccin	134	Isomaltose	63	0.558	0.857	37,475	0.647	30	111	13	128	110	3 original
4753	40 [680; 2,3-Dimethylsuccin	74	[912; Tetradecanoic acid (1TMS)]	64	0.554	0.846	18,464	0.616	31	109	17	124	28	13 original
4735	40 [680; 2,3-Dimethylsuccin	56	[829; Oleic acid (3TMS)]	64	0.551	0.777	35,554	0.574	32	110	38	103	101	43 original
11594	40 [680; 2,3-Dimethylsuccin	13	Uracil	64	0.544	0.825	37,356	0.621	33	108	25	116	108	10 original
4792	40 [680; 2,3-Dimethylsuccin	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	0.542	0.810	48,329	0.559	35	106	29	112	137	18 duplicate
4749	40 [680; 2,3-Dimethylsuccin	113	Galactose-6-phosphate	62	0.538	0.745	36,263	0.535	36	105	42	99	104	49 original
4791	40 [680; 2,3-Dimethylsuccin	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	0.536	0.572	16,923	0.468	37	104	57	84	26	96 original
11456	40 [680; 2,3-Dimethylsuccin	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.532	0.726	46,849	0.558	38	103	44	97	136	51 original
	40 [680; 2,3-Dimethylsuccin	12	Glyceric acid	63	0.528	0.802	40,732	0.552	39	102	33	108	117	56 duplicate
		129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]											
4808	40 [680; 2,3-Dimethylsuccin	132	[895; Isomaltose methoxyamine (8TMS)]	59	0.527	0.810	33,327	0.560	40	101	30	111	87	48 original
4811	40 [680; 2,3-Dimethylsuccin	88	Glucuronic acid	42	0.521	0.791	37,737	0.540	41	100	34	107	111	60 original
4767	40 [680; 2,3-Dimethylsuccin	110	Glucuronic acid	64	0.515	0.782	27,894	0.599	42	99	37	104	64	25 original
12086	40 [680; 2,3-Dimethylsuccin	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	0.513	0.787	19,831	0.556	43	98	35	106	35	53 duplicate
4764	40 [680; 2,3-Dimethylsuccin	85	[529; Methylcitric acid (4TMS)]	48	0.502	0.770	28,286	0.594	44	97	39	102	66	32 original
4799	40 [680; 2,3-Dimethylsuccin	120	[945; Uridine (3TMS)]	54	0.494	0.364	22,233	0.558	45	96	70	71	45	52 original
		57												
4736	40 [680; 2,3-Dimethylsuccin		[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55	0.494	0.770	28,020	0.574	46	95	40	101	67	44 original
12209	40 [680; 2,3-Dimethylsuccin	18	[590; 1-Acetyl-2-thiohydantoin]	64	0.491	0.700	29,392	0.492	47	94	48	93	69	87 duplicate
4793	40 [680; 2,3-Dimethylsuccin	114	Fructose-6-phosphate	53	0.486	0.746	34,982	0.554	48	93	41	100	96	55 original
10667	40 [680; 2,3-Dimethylsuccin	6	Glycerol	64	0.477	0.824	8,064	0.504	49	92	54	87	7	78 duplicate
		135												
4814	40 [680; 2,3-Dimethylsuccin		[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	0.474	0.660	23,423	0.452	50	91	52	89	48	105 original

4783	40 [680; 2,3-Dimethylsuccin	104 [795; Erythritol (4TMS)]	63 0,471	0,885	32,402	0,530	51	90	49	92	83	65 original
12331	40 [680; 2,3-Dimethylsuccin	19 Alanine (BP) (3TMS)	64 0,481	0,873	25,505	0,489	52	89	50	91	51	88 duplicate
4782	40 [680; 2,3-Dimethylsuccin	53 [NA]	55 0,436	0,701	38,336	0,519	53	88	47	94	112	72 original
4783	40 [680; 2,3-Dimethylsuccin	103 [648; Ethylamine (2TMS)]	63 0,391	0,585	30,750	0,505	54	87	55	86	74	77 original
4771	40 [680; 2,3-Dimethylsuccin	92 [680; Glycerol-2-phosphate (4TMS)]	54 0,377	0,584	31,860	0,454	55	86	56	85	79	103 original
4720	40 [680; 2,3-Dimethylsuccin	41 [639; Proline (2TMS)]	64 0,359	0,521	22,774	0,473	56	85	61	80	47	93 original
4802	40 [680; 2,3-Dimethylsuccin	123 [945; Galactofuranose-6-phosphate (7TMS)]	64 0,354	0,554	26,645	0,482	57	84	60	81	54	86 original
4807	40 [680; 2,3-Dimethylsuccin	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45 0,323	0,633	25,376	0,463	58	83	53	88	50	98 original
4766	40 [680; 2,3-Dimethylsuccin	87 [945; beta-D-Glucopyranose (5TMS)]	62 0,322	0,567	11,738	0,444	59	82	59	82	14	110 original
4780	40 [680; 2,3-Dimethylsuccin	101 [832; Dopamine (4TMS)]	64 0,315	0,434	31,773	0,454	60	81	67	74	78	104 original
4795	40 [680; 2,3-Dimethylsuccin	116 [882; Pseudouridine (5TMS)]	30 0,315	0,504	26,592	0,407	61	80	63	78	58	124 original
4788	40 [680; 2,3-Dimethylsuccin	109 Octadecanoic acid	64 0,309	0,664	19,805	0,540	62	79	51	90	34	59 original
4812	40 [680; 2,3-Dimethylsuccin	133 [855; Squalene]	64 0,299	0,287	31,886	0,377	63	78	74	67	80	132 original
4762	40 [680; 2,3-Dimethylsuccin	83 Sorbitol	58 0,298	-0,037	16,133	0,427	64	77	87	54	23	118 original
4790	40 [680; 2,3-Dimethylsuccin	111 [583; Erythritol (4TMS)]	42 0,282	0,423	44,742	0,375	65	76	68	73	131	133 original
4758	40 [680; 2,3-Dimethylsuccin	79 Glucose	64 0,277	0,515	7,520	0,536	66	75	62	79	5	62 original
4775	40 [680; 2,3-Dimethylsuccin	96 myo-Inositol	49 0,267	0,223	45,866	0,335	67	74	78	63	135	140 original
4806	40 [680; 2,3-Dimethylsuccin	127 [777; Fructose-6-phosphate methoxamine (6TMS)]	39 0,258	0,456	26,547	0,496	68	73	65	76	57	83 original
4773	40 [680; 2,3-Dimethylsuccin	94 Hexadecanoic acid	64 0,244	0,571	16,442	0,532	69	72	58	83	25	64 original
4778	40 [680; 2,3-Dimethylsuccin	99 [662; Ribose-5-phosphate methoxamine (BP) (5TMS)]	41 0,244	0,707	33,338	0,584	70	71	46	85	90	39 original
4770	40 [680; 2,3-Dimethylsuccin	91 [766; beta-D-Methylglucopyranoside (4TMS)]	64 0,234	0,342	33,412	0,456	71	70	71	70	91	102 original
4819	40 [680; 2,3-Dimethylsuccin	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49 0,223	0,328	42,058	0,417	72	69	72	69	124	120 original
4784	40 [680; 2,3-Dimethylsuccin	105 [705; 2-Ketogluconic acid (5TMS)]	48 0,218	0,487	26,413	0,497	73	68	64	77	56	82 original
4817	40 [680; 2,3-Dimethylsuccin	138 [674; Ergosterol (1TMS)]	46 0,208	0,320	41,596	0,387	74	67	73	68	122	130 original
4776	40 [680; 2,3-Dimethylsuccin	97 [756; beta-D-Methylglucopyranoside (4TMS)]	52 0,199	0,418	22,001	0,469	75	66	69	72	42	95 original
4759	40 [680; 2,3-Dimethylsuccin	80 [772; D-Glucose (5TMS)]	62 0,195	0,448	12,590	0,405	76	65	66	75	18	127 original
4743	40 [680; 2,3-Dimethylsuccin	64 [789; Tyramine (3TMS)]	63 0,178	0,272	33,649	0,353	77	64	76	65	93	139 original
4820	40 [680; 2,3-Dimethylsuccin	141 Lanosta-8,24-dien-3-beta-ol	61 0,156	0,283	42,793	0,442	78	63	75	68	125	111 original
1837	40 [680; 2,3-Dimethylsuccin	15 Alanine	64 0,141	0,244	19,030	0,556	79	62	77	64	31	54 duplicate
4816	40 [680; 2,3-Dimethylsuccin	137 Ergosterol	64 0,107	0,147	25,537	0,433	80	61	80	61	52	115 original
4763	40 [680; 2,3-Dimethylsuccin	84 Mannitol	62 0,087	0,199	12,397	0,495	81	60	79	62	17	84 original
4750	40 [680; 2,3-Dimethylsuccin	71 [731; Erythrose (3TMS)]	64 0,063	0,099	23,737	0,449	82	59	81	60	49	107 original
4803	40 [680; 2,3-Dimethylsuccin	124 [734; 1-Monooleoylglycerol (2TMS); 1-Monoheptadecanoylglycerol (1TMS)]	59 0,024	-0,095	52,809	0,428	83	58	88	53	140	117 original
4798	40 [680; 2,3-Dimethylsuccin	119 [931; myo-Inositol-2-phosphate (7TMS)]	64 -0,021	0,013	31,124	0,442	84	57	85	56	76	112 original
4772	40 [680; 2,3-Dimethylsuccin	93 [607; Putrescine (4TMS)]	60 -0,028	0,050	45,088	0,406	85	56	82	59	132	125 original
4732	40 [680; 2,3-Dimethylsuccin	53 Glycerol-2-phosphate	64 -0,029	-0,097	40,837	0,356	86	55	89	52	118	137 original
4797	40 [680; 2,3-Dimethylsuccin	118 [928; Glucopyranose-6-phosphate (6TMS)]	58 -0,033	0,017	35,246	0,371	87	54	83	58	98	134 original
4809	40 [680; 2,3-Dimethylsuccin	130 Trehalose	63 -0,033	-0,105	5,829	0,410	88	53	90	51	2	122 original
4769	40 [680; 2,3-Dimethylsuccin	90 [910; 9-(Z)-Hexadecanoic acid (1TMS)]	64 -0,035	-0,009	30,679	0,450	89	52	86	55	73	108 original
4786	40 [680; 2,3-Dimethylsuccin	107 9-(Z)-Octadecanoic acid	64 -0,063	-0,120	21,454	0,393	90	51	91	50	40	129 original
4818	40 [680; 2,3-Dimethylsuccin	139 [700; Ergosta-5,7-dien-3-ol]	38 -0,067	-0,155	41,442	0,357	91	50	94	47	121	136 original
4726	40 [680; 2,3-Dimethylsuccin	47 [NA]	64 -0,070	-0,136	33,602	0,499	92	49	93	48	92	81 original
4737	40 [680; 2,3-Dimethylsuccin	58 [636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64 -0,117	-0,204	22,090	0,430	93	48	95	46	44	116 original
14252	40 [680; 2,3-Dimethylsuccin	36 [596; N-Acetylglutamic acid (2TMS)]	64 -0,121	-0,233	10,057	0,458	94	47	96	45	11	100 duplicate
4754	40 [680; 2,3-Dimethylsuccin	75 Lysine	64 -0,154	-0,282	8,178	0,439	95	46	98	43	8	113 original
10601	40 [680; 2,3-Dimethylsuccin	7 Threonine	64 -0,155	-0,287	6,278	0,438	96	45	99	42	3	114 duplicate
9982	40 [680; 2,3-Dimethylsuccin	1 [938; Sulfuric acid (2TMS)]	38 -0,162	-0,016	27,855	0,545	97	44	84	57	62	57 duplicate
10396	40 [680; 2,3-Dimethylsuccin	4 Phosphoric acid	51 -0,169	-0,252	5,541	0,396	98	43	97	44	1	128 duplicate
4745	40 [680; 2,3-Dimethylsuccin	66 Glycetic acid-3-phosphate	64 -0,195	-0,345	35,476	0,518	99	42	105	36	100	74 original

4739	40	[680; 2,3-Dimethylsuccin]	60	Glycerol-3-phosphate	64	-0.211	-0.287	14.631	0.447	100	41	100	41	21	108	original
4815	40	[680; 2,3-Dimethylsuccin]	138	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.221	-0.129	17.487	0.354	101	40	92	49	27	138	original
4746	40	[680; 2,3-Dimethylsuccin]	67	Citric acid	64	-0.225	-0.300	11.478	0.384	102	39	101	40	13	131	original
4787	40	[680; 2,3-Dimethylsuccin]	108	Octadecanoic acid	64	-0.234	-0.312	35.965	0.405	103	38	102	39	103	128	original
4751	40	[680; 2,3-Dimethylsuccin]	72	[918; D-Xylopyranose (4TMS)]	63	-0.253	-0.338	36.493	0.365	104	37	104	37	105	135	original
10121	40	[680; 2,3-Dimethylsuccin]	2	Serine	62	-0.305	-0.401	25.553	0.445	105	36	107	34	53	109	tuplicate
13717	40	[680; 2,3-Dimethylsuccin]	31	[622; Parabanic acid (2TMS)]	64	-0.311	-0.560	40.188	0.530	106	35	111	30	118	67	tuplicate
14356	40	[680; 2,3-Dimethylsuccin]	37	Phenylalanine	64	-0.321	-0.452	12.862	0.417	107	34	109	32	19	121	tuplicate
10934	40	[680; 2,3-Dimethylsuccin]	8	Isoleucine	55	-0.335	-0.321	22.451	0.409	108	33	103	38	48	123	tuplicate
11066	40	[680; 2,3-Dimethylsuccin]	9	Proline	63	-0.338	-0.438	20.419	0.460	109	32	108	33	38	99	tuplicate
13271	40	[680; 2,3-Dimethylsuccin]	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	-0.344	-0.769	42.852	0.597	110	31	131	10	128	29	tuplicate
4740	40	[680; 2,3-Dimethylsuccin]	61	[NA]	64	-0.362	-0.391	32.498	0.418	111	30	106	35	85	119	original
4731	40	[680; 2,3-Dimethylsuccin]	52	[NA]	46	-0.376	-0.636	43.095	0.606	112	29	118	23	127	23	original
10259	40	[680; 2,3-Dimethylsuccin]	3	Ethanolamine	82	-0.380	-0.568	39.608	0.528	113	28	113	28	115	68	tuplicate
4742	40	[680; 2,3-Dimethylsuccin]	63	Glutamine	52	-0.382	-0.632	37.445	0.575	114	27	117	24	109	42	original
4777	40	[680; 2,3-Dimethylsuccin]	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	48	-0.392	-0.741	44.186	0.561	115	26	127	14	130	47	original
12809	40	[680; 2,3-Dimethylsuccin]	23	Homoserine	64	-0.395	-0.789	32.267	0.598	116	25	133	8	82	26	tuplicate
4722	40	[680; 2,3-Dimethylsuccin]	43	[548; Leucine (2TBS)]	60	-0.403	-0.566	28.618	0.476	117	24	112	29	70	92	original
12452	20	[618; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.419	31	-0.419	-0.746	33.853	0.626	118	23	129	12	94	9	tuplicate
4738	40	[680; 2,3-Dimethylsuccin]	59	Omithine; Arginine	64	-0.434	-0.547	9.566	0.465	119	22	110	31	10	97	original
13826	40	[680; 2,3-Dimethylsuccin]	32	[728; N,N-Dimethyllysine methyl ester]	63	-0.455	-0.695	41.925	0.598	120	21	123	18	123	27	tuplicate
4760	40	[680; 2,3-Dimethylsuccin]	81	Tyrosine	64	-0.464	-0.824	12.395	0.615	121	20	116	25	16	16	original
14041	40	[680; 2,3-Dimethylsuccin]	34	Aspartic acid	64	-0.474	-0.620	9.476	0.493	122	19	115	26	9	85	tuplicate
4730	40	[680; 2,3-Dimethylsuccin]	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.482	-0.711	43.810	0.503	123	18	125	16	128	79	tuplicate
4747	40	[680; 2,3-Dimethylsuccin]	68	[570; Hypoxanthine (2TMS)]	20	-0.484	-0.858	30.818	0.558	124	17	138	3	75	50	original
4727	40	[680; 2,3-Dimethylsuccin]	48	Asparagine	64	-0.489	-0.750	33.327	0.574	125	16	130	11	88	45	original
4756	40	[680; 2,3-Dimethylsuccin]	77	[826; beta-[(5-methyl-2-phenylmethyl)amino]-benzoic acid methyl ester]	62	-0.490	-0.617	16.275	0.486	126	15	114	27	24	89	original
4774	40	[680; 2,3-Dimethylsuccin]	95	[770; 3,4,6-Trisubstituted phenylethanolamine (5TMS)]	50	-0.496	-0.686	45.437	0.472	127	14	122	19	133	94	original
4734	40	[680; 2,3-Dimethylsuccin]	55	[612; 4-Aminobutyric acid (2TBS)]	43	-0.506	-0.655	45.619	0.519	128	13	120	21	134	73	original
13934	40	[680; 2,3-Dimethylsuccin]	33	Methionine	64	-0.517	-0.704	32.461	0.517	129	12	124	17	84	75	tuplicate
13607	40	[680; 2,3-Dimethylsuccin]	30	[815; Ethyl-3(2H)-thiophenone]	64	-0.527	-0.640	13.988	0.456	130	11	119	22	20	101	tuplicate
11197	40	[680; 2,3-Dimethylsuccin]	10	Glycine	64	-0.529	-0.808	19.998	0.596	131	10	135	6	36	31	tuplicate
13042	40	[680; 2,3-Dimethylsuccin]	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.534	-0.811	37.253	0.586	132	9	136	5	106	38	tuplicate
4810	40	[680; 2,3-Dimethylsuccin]	131	[626; 5-Methylthioadenosine (3TMS)]	55	-0.538	-0.717	44.119	0.480	133	8	126	15	129	90	original
4768	40	[680; 2,3-Dimethylsuccin]	69	Arginine	60	-0.540	-0.827	20.211	0.596	134	7	137	4	37	30	original
4721	40	[680; 2,3-Dimethylsuccin]	89	[775; Dopamine (4TMS)]	35	-0.550	-0.789	33.957	0.539	135	6	134	7	95	61	original
4724	40	[680; 2,3-Dimethylsuccin]	42	Glutamic acid	60	-0.566	-0.686	19.248	0.480	136	5	121	20	33	91	original
10532	40	[680; 2,3-Dimethylsuccin]	45	Homocysteine	61	-0.573	-0.776	51.190	0.519	137	4	132	9	139	71	original
4728	40	[680; 2,3-Dimethylsuccin]	5	Leucine	45	-0.584	-0.864	32.108	0.633	138	3	139	2	81	7	tuplicate
4761	40	[680; 2,3-Dimethylsuccin]	49	[877; Pyrophosphoric acid (4TMS)]	64	-0.597	-0.741	49.030	0.499	139	2	128	13	138	80	original
12332	41	[639; Proline (2TMS)]	82	Lysine	39	-0.684	-0.937	20.482	0.655	140	1	140	1	39	2	original
4893	41	[639; Proline (2TMS)]	19	Alanine (BP) (3TMS)	64	-0.759	0.932	3.630	0.658	141	140	1	140	1	1	tuplicate
4893	41	[639; Proline (2TMS)]	114	Fructose-6-phosphate	53	-0.566	0.701	14.617	0.552	2	139	3	138	63	9	original
13156	41	[639; Proline (2TMS)]	123	[945; Galactofuranose-6-phosphate (7TMS)]	64	-0.547	0.744	4.591	0.561	3	138	2	139	3	4	original
4892	41	[639; Proline (2TMS)]	26	Citramalic acid	64	-0.494	0.666	5.366	0.498	4	137	5	136	6	25	tuplicate
4892	41	[639; Proline (2TMS)]	113	Galactose-6-phosphate	62	-0.485	0.648	14.826	0.521	5	136	7	134	67	13	original
4885	41	[639; Proline (2TMS)]	108	[733; Threitol (4TMS)]	62	-0.482	0.657	10.316	0.555	6	135	8	135	25	8	original
4883	41	[639; Proline (2TMS)]	104	[795; Erythritol (4TMS)]	63	-0.477	0.586	11.226	0.520	7	134	20	121	33	14	original
4894	41	[639; Proline (2TMS)]	115	Glucose-6-phosphate	62	-0.439	0.639	13.009	0.473	8	133	9	132	45	53	original

4852	41 [639; Proline (2TMS)]	73 [708; Glucose methoxyamine (5TMS)]	57 0.424	0.589	15,398	0.416	9	132	19	122	70	107 original
4900	41 [639; Proline (2TMS)]	121 [657; Erythritol (4TMS)]	55 0.415	0.642	20,965	0.502	10	131	8	133	101	21 original
4859	41 [639; Proline (2TMS)]	80 [772; D-Glucose (5TMS)]	62 0.414	0.634	19,143	0.471	11	130	11	130	91	55 original
4897	41 [639; Proline (2TMS)]	118 [928; Glucopyranose-6-phosphate (6TMS)]	58 0.407	0.813	14,416	0.420	12	128	17	124	60	103 original
12210	41 [639; Proline (2TMS)]	18 [590; 1-Acetyl-2-thiohydantoin]	64 0.408	0.623	8,001	0.431	13	128	13	128	15	93 duplicate
4896	41 [639; Proline (2TMS)]	117 [724; Glyceral (3TMS)]	56 0.404	0.616	13,221	0.483	14	127	16	125	46	45 original
4895	41 [639; Proline (2TMS)]	116 [882; Pseudouridine (5TMS)]	30 0.402	0.255	13,460	0.293	15	126	67	74	49	137 original
4849	41 [639; Proline (2TMS)]	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57 0.401	0.533	8,182	0.464	16	125	28	113	18	59 original
4866	41 [639; Proline (2TMS)]	87 [945; beta-D-Glucopyranose (5TMS)]	62 0.399	0.673	23,445	0.500	17	124	4	137	119	22 original
14148	41 [639; Proline (2TMS)]	35 Pyroglutamic acid	64 0.399	0.626	29,398	0.499	18	123	12	129	136	23 duplicate
4855	41 [639; Proline (2TMS)]	76 Fructose	64 0.371	0.635	14,414	0.494	19	122	10	131	59	31 original
4858	41 [639; Proline (2TMS)]	79 Glucose	64 0.360	0.568	23,056	0.480	20	121	24	117	118	47 original
14663	41 [639; Proline (2TMS)]	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	64 0.359	0.521	22,774	0.473	21	120	32	109	115	52 duplicate
4857	41 [639; Proline (2TMS)]	78 Mannose	62 0.357	0.578	16,524	0.491	22	119	23	118	76	34 original
12573	41 [639; Proline (2TMS)]	21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64 0.354	0.537	5,719	0.440	23	118	26	115	7	82 duplicate
4901	41 [639; Proline (2TMS)]	122 [644; Erythritol (4TMS)]	52 0.348	0.519	22,506	0.498	24	117	33	108	11	24 original
4911	41 [639; Proline (2TMS)]	132 [895; Isomaltose methoxyamine (8TMS)]	42 0.347	0.415	21,473	0.423	25	116	52	89	104	89 original
11712	41 [639; Proline (2TMS)]	14 Fumaric acid	64 0.347	0.534	16,908	0.459	26	115	27	114	80	82 duplicate
4904	41 [639; Proline (2TMS)]	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64 0.344	0.620	20,223	0.479	27	114	14	127	98	48 original
12692	41 [639; Proline (2TMS)]	22 [890; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52 0.344	0.516	19,110	0.401	28	113	35	106	90	116 duplicate
13385	41 [639; Proline (2TMS)]	28 Malic acid	64 0.343	0.517	6,456	0.483	29	112	34	107	8	44 duplicate
4889	41 [639; Proline (2TMS)]	110 [715; Erythritol (4TMS)]	54 0.336	0.609	17,038	0.558	30	111	18	123	81	5 original
11838	41 [639; Proline (2TMS)]	15 Alanine	64 0.333	0.481	7,980	0.455	31	110	39	102	14	65 duplicate
4853	41 [639; Proline (2TMS)]	74 [912; Tetradecanoic acid (1TMS)]	64 0.323	0.617	14,453	0.503	32	109	15	126	61	20 original
4841	41 [639; Proline (2TMS)]	62 [812; D-Xylofuranose (4TMS)]	64 0.320	0.526	4,546	0.496	33	108	30	111	2	28 original
4862	41 [639; Proline (2TMS)]	83 Sorbitol	58 0.312	0.162	11,575	0.347	34	107	78	63	34	134 original
4917	41 [639; Proline (2TMS)]	138 [674; Ergosterol (1TMS)]	46 0.302	0.543	22,688	0.435	35	106	25	116	114	89 original
4864	41 [639; Proline (2TMS)]	85 [528; Methylcitric acid (4TMS)]	48 0.301	0.499	10,423	0.421	36	105	37	104	27	102 original
4912	41 [639; Proline (2TMS)]	133 [855; Squalene]	64 0.297	0.395	10,943	0.443	37	104	53	88	31	78 original
4865	41 [639; Proline (2TMS)]	86 [793; D-Galactono-1,4-lactone (4TMS)]	61 0.295	0.582	16,688	0.472	38	103	21	120	77	54 original
10668	41 [639; Proline (2TMS)]	6 Glyceral	64 0.291	0.504	29,999	0.488	39	102	36	105	138	36 duplicate
4905	41 [639; Proline (2TMS)]	126 [559; Erythritol (4TMS)]	45 0.289	0.530	13,924	0.556	40	101	29	112	53	7 original
4843	41 [639; Proline (2TMS)]	64 [789; Tyramine (3TMS)]	63 0.278	0.294	12,359	0.394	41	100	63	78	40	120 original
11328	41 [639; Proline (2TMS)]	11 Succinic acid	64 0.278	0.454	8,306	0.409	42	99	44	97	17	112 duplicate
4875	41 [639; Proline (2TMS)]	96 myo-Inositol	49 0.262	0.264	26,647	0.287	43	98	66	75	130	138 original
14460	41 [639; Proline (2TMS)]	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	64 0.255	0.444	8,910	0.414	44	97	45	96	21	108 duplicate
4915	41 [639; Proline (2TMS)]	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17 0.235	0.358	7,699	0.289	45	96	59	82	11	140 original
4867	41 [639; Proline (2TMS)]	88 Gluconic acid	64 0.235	0.422	9,756	0.506	46	95	50	91	22	18 original
11585	41 [639; Proline (2TMS)]	13 Uracil	64 0.232	0.428	8,384	0.493	47	94	46	95	18	33 duplicate
4835	41 [639; Proline (2TMS)]	56 [829; Orotic acid (3TMS)]	64 0.229	0.490	16,852	0.488	48	93	40	101	79	35 original
4891	41 [639; Proline (2TMS)]	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63 0.226	0.426	25,003	0.456	49	92	49	92	123	64 original
4878	41 [639; Proline (2TMS)]	100 [857; Mannitol (6TMS)]	64 0.223	0.230	7,729	0.410	50	91	71	70	12	111 original
4919	41 [639; Proline (2TMS)]	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49 0.223	0.302	22,800	0.404	51	90	62	79	117	114 original
4829	41 [639; Proline (2TMS)]	50 [746; Ribonic acid-1,4-lactone (3TMS)]	61 0.212	0.390	27,010	0.424	52	89	54	87	131	98 original
4899	41 [639; Proline (2TMS)]	120 [945; Uridine (3TMS)]	54 0.212	0.096	6,668	0.451	53	88	83	58	9	68 original
4868	41 [639; Proline (2TMS)]	109 Octadecanoic acid	64 0.197	0.582	12,605	0.496	54	87	22	119	43	27 original
14562	41 [639; Proline (2TMS)]	39 [829; 1-Phenylethanol (1TMS)]	63 0.196	0.416	11,794	0.443	55	86	51	90	36	79 duplicate
11963	41 [639; Proline (2TMS)]	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	64 0.192	0.379	7,890	0.504	56	85	55	86	13	19 duplicate
4880	41 [639; Proline (2TMS)]	101 [832; Dopamine (4TMS)]	64 0.190	0.161	13,267	0.413	57	84	80	61	47	109 original
4881	41 [639; Proline (2TMS)]	102 [904; Galactose methoxyamine (5TMS)]	64 0.189	0.201	14,114	0.429	58	83	73	68	55	94 original
12927	41 [639; Proline (2TMS)]	24 [725; 2-Keibocanoic acid (2TMS)]	64 0.188	0.427	20,580	0.488	59	82	47	84	100	39 duplicate

4882	41 [639; Proline (2TMS)]	103 [648; Ethylamine (2TMS)]	63 0.188	0.236	14,584	0.444	60	81	68	73	62	76 original
12087	41 [639; Proline (2TMS)]	17 [700; 2-methyl-1,2-propanediol (2TMS)]	64 0.188	0.377	8,501	0.431	61	80	58	85	20	92 duplicate
4825	41 [639; Proline (2TMS)]	46. Arabinose	64 0.186	0.497	13,738	0.488	62	79	38	103	51	37 original
4823	41 [639; Proline (2TMS)]	44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	50 0.184	0.281	12,299	0.478	63	78	64	77	39	49 original
135		135										
4914	41 [639; Proline (2TMS)]	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64 0.177	0.362	4,859	0.444	64	77	57	84	4	75 original
13497	41 [639; Proline (2TMS)]	29 Erythritol	64 0.174	0.345	12,006	0.442	65	76	60	81	38	80 duplicate
4906	41 [639; Proline (2TMS)]	127 [777; Fructose-6-phosphate methoxyamine (5TMS)]	39 0.171	0.280	10,388	0.422	66	75	65	78	26	100 original
4913	41 [639; Proline (2TMS)]	134 Isomaltose	64 0.171	0.485	15,785	0.484	67	74	41	100	73	43 original
58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]											
4837	41 [639; Proline (2TMS)]	65 [646; 3-Deoxyglucitol (5TMS)]	64 0.169	0.181	8,391	0.377	68	73	75	66	19	126 original
4844	41 [639; Proline (2TMS)]	94 Hexadecanoic acid	63 0.168	0.469	18,241	0.517	69	72	42	98	86	16 original
4873	41 [639; Proline (2TMS)]	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	64 0.161	0.522	10,637	0.533	70	71	31	110	28	10 original
4908	41 [639; Proline (2TMS)]	Glc]	59 0.156	0.465	14,722	0.523	71	70	43	98	65	12 original
11457	41 [639; Proline (2TMS)]	12 Glycercic acid	63 0.151	0.320	19,323	0.417	72	69	61	80	93	105 duplicate
4851	41 [639; Proline (2TMS)]	72 [919; D-Xylopyranose (4TMS)]	63 0.148	0.198	15,635	0.365	73	68	74	67	72	128 original
4818	41 [639; Proline (2TMS)]	139 [700; Ergosta-5,7-dien-3-ol]	38 0.115	0.175	24,510	0.324	74	67	76	65	121	135 original
4890	41 [639; Proline (2TMS)]	111 [583; Erythritol (4TMS)]	42 0.106	0.231	27,329	0.447	75	66	70	71	132	72 original
4920	41 [639; Proline (2TMS)]	141 Lanosta-8,24-dien-3-beta-ol	61 0.102	0.161	21,853	0.453	76	65	79	62	106	67 original
4833	41 [639; Proline (2TMS)]	54 [NA]	55 0.098	0.235	19,720	0.443	77	64	69	72	96	77 original
4850	41 [639; Proline (2TMS)]	71 [731; Erythrose (3TMS)]	64 0.093	0.207	5,255	0.437	78	63	72	69	5	87 original
4870	41 [639; Proline (2TMS)]	91 [766; beta-D-Methylglucopyranoside (4TMS)]	64 0.077	0.046	18,704	0.468	79	62	87	54	88	57 original
4871	41 [639; Proline (2TMS)]	92 [680; Glycerol-2-phosphate (4TMS)]	54 0.075	0.427	13,409	0.442	80	61	48	93	48	81 original
4854	41 [639; Proline (2TMS)]	75 Lysine	64 0.072	0.109	28,221	0.385	81	60	81	60	133	122 original
14253	41 [639; Proline (2TMS)]	36 [596; N-Acetylglutamic acid (2TMS)]	64 0.071	0.079	17,702	0.394	82	59	85	56	84	119 duplicate
4916	41 [639; Proline (2TMS)]	137 Ergosterol	64 0.062	0.102	10,161	0.382	83	58	82	59	24	123 original
4909	41 [639; Proline (2TMS)]	130 Trehalose	63 0.060	0.064	16,593	0.357	84	57	86	55	87	132 original
10397	41 [639; Proline (2TMS)]	4 Phosphoric acid	51 0.042	0.023	22,597	0.276	85	56	89	52	113	139 duplicate
4826	41 [639; Proline (2TMS)]	47 [NA]	64 0.017	0.021	14,893	0.426	86	55	90	51	64	96 original
57												
4836	41 [639; Proline (2TMS)]	[757; 2-Desoxy-pentose-3-ylose dimethoxyamine (2TMS)]	55 0.017	0.359	14,114	0.477	87	54	58	83	54	50 original
4839	41 [639; Proline (2TMS)]	60 Glycerol-3-phosphate	64 0.003	0.004	10,855	0.573	88	53	92	49	29	3 original
4907	41 [639; Proline (2TMS)]	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45 -0.002	0.086	10,108	0.437	89	52	84	57	23	88 original
4903	41 [639; Proline (2TMS)]	124 [734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]	59 -0.017	0.000	31,937	0.357	90	51	93	48	140	131 original
10802	41 [639; Proline (2TMS)]	7 Threonine	64 -0.069	0.009	18,827	0.378	91	50	91	50	89	125 duplicate
4876	41 [639; Proline (2TMS)]	97 [756; beta-D-Methylglucopyranoside (4TMS)]	52 -0.074	0.028	16,202	0.495	92	49	88	53	75	30 original
4845	41 [639; Proline (2TMS)]	66 Glycercic acid-3-phosphate	64 -0.078	-0.076	14,316	0.438	93	48	96	45	57	84 original
10122	41 [639; Proline (2TMS)]	2 Serine	62 -0.111	-0.021	14,756	0.381	94	47	94	47	68	124 duplicate
4898	41 [639; Proline (2TMS)]	119 [931; myo-Inositol-2-phosphate (7TMS)]	64 -0.114	-0.110	11,646	0.464	95	46	97	44	35	58 original
4878	41 [639; Proline (2TMS)]	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41 -0.141	0.169	17,046	0.446	96	45	77	64	82	73 original
4884	41 [639; Proline (2TMS)]	105 [705; 2-Ketogluconic acid (5TMS)]	48 -0.144	-0.197	13,605	0.460	97	44	105	36	50	61 original
4846	41 [639; Proline (2TMS)]	67 Citric acid	64 -0.146	-0.134	12,715	0.461	98	43	99	42	44	60 original
13827	41 [639; Proline (2TMS)]	32 [729; N,N-Dimethyllysine methyl ester]	63 -0.150	-0.178	22,782	0.484	99	42	102	39	116	41 duplicate
4886	41 [639; Proline (2TMS)]	107 9-(Z)-Octadecenoic acid	64 -0.152	-0.207	6,925	0.454	100	41	106	35	10	66 original
4863	41 [639; Proline (2TMS)]	84 Mannitol	62 -0.155	-0.221	22,534	0.420	101	40	109	32	112	104 original
13272	41 [639; Proline (2TMS)]	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53 -0.163	-0.440	25,754	0.402	102	39	123	18	127	115 duplicate
4869	41 [639; Proline (2TMS)]	90 [910; 9-(Z)-Hexadecanoic acid (1TMS)]	64 -0.164	-0.265	10,940	0.427	103	38	112	29	30	95 original
4887	41 [639; Proline (2TMS)]	108 Octadecanoic acid	64 -0.167	-0.154	15,127	0.361	104	37	101	40	69	129 original
14357	41 [639; Proline (2TMS)]	37 Phenylalanine	64 -0.173	-0.138	11,929	0.488	105	36	100	41	37	38 duplicate

4877	41 [639; Proline (2TMS)]	98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	48 -0.204	-0.384	25.494	0.458	108	35	121	20	125	63 original
4882	41 [639; Proline (2TMS)]	43 [548; Leucine (2TBS)]	60 -0.214	-0.382	11.188	0.435	107	34	120	21	32	90 original
4860	41 [639; Proline (2TMS)]	81 Tyrosine	64 -0.222	-0.308	24.241	0.516	108	33	114	27	120	17 original
4832	41 [639; Proline (2TMS)]	53 Glyceral-2-phosphate	64 -0.227	-0.366	19.581	0.425	109	32	117	24	95	97 original
10260	41 [639; Proline (2TMS)]	3 Ethanolamine	62 -0.231	-0.382	19.388	0.487	110	31	119	22	94	28 duplicate
4838	41 [639; Proline (2TMS)]	59 Ornithine; Arginine	64 -0.231	-0.193	29.798	0.361	111	30	103	38	137	130 original
11067	41 [639; Proline (2TMS)]	9 Proline	63 -0.235	-0.075	20.105	0.398	112	29	95	46	97	117 duplicate
13718	41 [639; Proline (2TMS)]	31 [622; Parabanic acid (2TMS)]	64 -0.247	-0.357	19.278	0.431	113	28	118	25	92	91 duplicate
9983	41 [639; Proline (2TMS)]	1 [938; Sulfuric acid (2TMS)]	36 -0.248	-0.234	13.924	0.487	114	27	110	31	52	40 duplicate
4856	41 [639; Proline (2TMS)]	77 [826; beta-[[[5-methyl-2-thienyl]methyleneamino- benzeneacetic acid methyl ester]	62 -0.254	-0.219	21.143	0.408	115	26	108	33	103	113 original
4821	41 [639; Proline (2TMS)]	42 Glutamic acid	60 -0.329	-0.219	22.256	0.347	116	24	107	34	107	133 original
4872	41 [639; Proline (2TMS)]	93 [607; Putrescine (4TMS)]	60 -0.329	-0.352	25.188	0.368	117	25	115	26	124	127 original
13935	41 [639; Proline (2TMS)]	33 Methionine	64 -0.330	-0.259	14.343	0.437	118	23	111	30	58	85 duplicate
14042	41 [639; Proline (2TMS)]	34 Aspartic acid	64 -0.333	-0.271	22.344	0.412	119	21	113	28	108	110 duplicate
12810	41 [639; Proline (2TMS)]	23 Homoserine	64 -0.333	-0.524	14.947	0.480	120	22	126	15	68	48 duplicate
13043	41 [639; Proline (2TMS)]	25 [709; 2,5-Diaminovalerolactam (2TMS)]	48 -0.337	-0.381	21.660	0.437	121	20	118	23	105	86 duplicate
4848	41 [639; Proline (2TMS)]	69 Arginine	60 -0.344	-0.411	15.417	0.475	122	19	122	19	71	51 original
13608	41 [639; Proline (2TMS)]	30 [815; Ethyl-3(2H)-thiophenone]	64 -0.350	-0.195	20.362	0.393	123	17	104	37	99	121 duplicate
11198	41 [639; Proline (2TMS)]	10 Glycine	64 -0.350	-0.560	12.586	0.496	124	18	127	14	42	29 duplicate
4824	41 [639; Proline (2TMS)]	45 Homocysteine	61 -0.373	-0.468	30.033	0.416	125	16	124	17	139	106 original
4827	41 [639; Proline (2TMS)]	48 Asparagine	64 -0.400	-0.639	16.711	0.484	126	15	132	9	78	42 original
10935	41 [639; Proline (2TMS)]	8 Isoleucine	55 -0.414	-0.131	14.280	0.320	127	13	98	43	56	136 duplicate
4910	41 [639; Proline (2TMS)]	131 [828; 5-Methylthioadenosine (3TMS)]	55 -0.414	-0.709	24.848	0.574	128	14	136	5	122	2 original
4828	41 [639; Proline (2TMS)]	49 [877; Pyrophosphoric acid (4TMS)]	64 -0.421	-0.589	29.177	0.445	129	12	128	13	134	74 original
4834	41 [639; Proline (2TMS)]	55 [612; 4-Aminobutyric acid (2TBS)]	43 -0.464	-0.710	29.229	0.448	130	11	137	4	135	71 original
4874	41 [639; Proline (2TMS)]	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50 -0.466	-0.601	25.965	0.557	131	10	129	12	128	6 original
4840	41 [639; Proline (2TMS)]	61 [NA]	64 -0.483	-0.613	12.502	0.471	132	9	131	10	41	56 original
12453	41 [639; Proline (2TMS)]	20 [619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	31 -0.488	-0.803	21.098	0.532	133	8	140	1	102	11 duplicate
4847	41 [639; Proline (2TMS)]	68 [570; Hypoxanthine (2TMS)]	20 -0.485	-0.704	18.081	0.438	134	7	134	7	85	83 original
4830	41 [639; Proline (2TMS)]	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44 -0.499	-0.497	26.610	0.448	135	6	125	16	129	70 original
4831	41 [639; Proline (2TMS)]	52 [NA]	46 -0.530	-0.707	25.637	0.518	136	5	135	6	128	15 original
4861	41 [639; Proline (2TMS)]	82 Lysine	39 -0.533	-0.748	16.036	0.493	137	4	139	2	74	32 original
4842	41 [639; Proline (2TMS)]	63 Glutamine	52 -0.573	-0.672	22.480	0.422	138	3	133	8	110	101 original
10533	41 [639; Proline (2TMS)]	5 Leucine	45 -0.634	-0.609	17.274	0.397	139	2	130	11	83	118 duplicate
4868	41 [639; Proline (2TMS)]	89 [775; Dopamine (4TMS)]	35 -0.637	-0.747	22.395	0.450	140	1	138	3	109	69 original
4959	41 [639; Proline (2TMS)]	81 Tyrosine	60 -0.800	0.860	11.476	0.550	1	140	9	132	6	17 original
13609	42 Glutamic acid	30 [815; Ethyl-3(2H)-thiophenone]	60 0.779	0.939	9.652	0.618	2	139	2	139	3	5 duplicate
4955	42 Glutamic acid	77 [826; beta-[[[5-methyl-2-thienyl]methyleneamino- benzeneacetic acid methyl ester]	59 0.766	0.920	7.366	0.570	3	138	4	137	1	12 original
4947	42 Glutamic acid	69 Arginine	59 0.753	0.911	10.176	0.593	4	137	5	136	5	7 original
4929	42 Glutamic acid	51 [498; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44 0.746	0.859	42.264	0.621	5	136	10	131	136	3 original
4937	42 Glutamic acid	59 Ornithine; Arginine	60 0.740	0.931	19.492	0.619	6	135	3	138	25	4 original
11199	42 Glutamic acid	10 Glycine	60 0.728	0.791	13.704	0.461	7	134	16	125	9	64 duplicate
4960	42 Glutamic acid	82 Lysine	38 0.710	0.799	15.061	0.571	8	133	15	126	17	11 original
13936	42 Glutamic acid	33 Methionine	60 0.710	0.887	22.369	0.592	9	132	6	135	40	8 duplicate
10534	42 Glutamic acid	5 Leucine	44 0.702	0.855	29.872	0.652	10	131	11	130	87	1 duplicate
13928	42 Glutamic acid	32 [729; N,N-Dimethyllysine methyl ester]	60 0.698	0.863	29.434	0.643	11	130	1	140	82	2 duplicate
10261	42 Glutamic acid	3 Ethanolamine	59 0.695	0.744	31.614	0.459	12	129	22	119	97	66 duplicate

12454	42	Glutamic acid	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	0.690	0.654	34.981	0.599	13	128	30	111	115	6 duplicate
14358	42	Glutamic acid	37	Phenylalanine	60	0.636	0.946	14.231	0.535	15	127	12	129	11	23 duplicate
4833	42	Glutamic acid	55	[612; 4-Aminobutyric acid (2TBS)]	42	0.633	0.583	44.356	0.569	15	126	33	108	139	13 original
4926	42	Glutamic acid	48	Asparagine	60	0.620	0.652	24.452	0.500	16	125	31	110	52	37 original
14043	42	Glutamic acid	34	Aspartic acid	60	0.609	0.809	13.834	0.568	17	124	14	127	10	14 duplicate
11068	42	Glutamic acid	59	Proline	59	0.594	0.868	8.001	0.563	18	123	7	134	2	15 duplicate
5009	42	Glutamic acid	131	[626; 5-Methylthioadenosine (3TMS)]	51	0.591	0.408	37.694	0.434	19	122	44	97	126	76 original
4946	42	Glutamic acid	68	[570; Hypoxanthine (2TMS)]	19	0.567	0.864	28.072	0.547	20	121	8	133	75	19 original
10936	42	Glutamic acid	8	Isoleucine	54	0.561	0.765	15.708	0.507	21	120	19	122	19	33 duplicate
4945	42	Glutamic acid	67	Citric acid	60	0.542	0.689	15.031	0.450	22	119	27	114	16	70 original
13719	42	Glutamic acid	31	[622; Parabenic acid (2TMS)]	60	0.540	0.749	32.367	0.495	23	118	21	120	101	43 duplicate
4973	42	Glutamic acid	95	[770; 3,4,6-Trisubstitutedphenylmethanolamine (5TMS)]	48	0.532	0.493	40.520	0.418	24	117	38	103	133	85 original
4938	42	Glutamic acid	60	Glycerol-3-phosphate	60	0.521	0.687	14.432	0.461	25	116	28	113	13	65 original
10123	42	Glutamic acid	2	Serine	60	0.506	0.824	14.823	0.552	26	115	13	128	15	16 duplicate
4923	42	Glutamic acid	45	Homocysteine	57	0.503	0.550	43.615	0.493	27	114	37	104	136	45 original
5014	42	Glutamic acid	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.485	0.580	9.926	0.220	28	113	34	107	4	139 original
4927	42	Glutamic acid	49	[877; Pyrophosphoric acid (4TMS)]	60	0.485	0.435	40.195	0.365	29	112	42	99	132	114 original
4967	42	Glutamic acid	89	[775; Dopamine (4TMS)]	35	0.449	0.561	30.680	0.530	30	111	35	106	91	26 original
13044	42	Glutamic acid	25	[709; 2,5-Diaminovalerolactam (2TMS)]	44	0.431	0.707	23.339	0.416	31	110	25	116	43	89 duplicate
10803	42	Glutamic acid	7	Threonine	60	0.428	0.785	14.538	0.541	32	109	18	123	14	21 duplicate
4939	42	Glutamic acid	61	[NA]	60	0.427	0.294	27.348	0.392	33	108	51	90	72	98 original
12811	42	Glutamic acid	23	Homoserine	60	0.423	0.736	23.493	0.546	34	107	23	118	45	20 duplicate
4986	42	Glutamic acid	108	Octadecenoic acid	60	0.395	0.491	28.770	0.396	35	106	39	102	85	94 original
4944	42	Glutamic acid	66	Glyceric acid-3-phosphate	60	0.394	0.682	29.124	0.467	36	105	29	112	80	61 original
4976	42	Glutamic acid	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	46	0.378	0.703	37.220	0.548	37	104	26	115	125	18 original
4953	42	Glutamic acid	75	Lysine	60	0.351	0.754	18.948	0.523	38	103	20	121	22	28 original
13273	42	Glutamic acid	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	52	0.345	0.787	36.021	0.581	39	102	17	124	122	9 duplicate
4930	42	Glutamic acid	52	[NA]	43	0.282	0.390	34.650	0.494	40	101	45	96	111	44 original
4936	42	Glutamic acid	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	60	0.279	0.707	16.756	0.499	41	100	24	117	20	39 original
14254	42	Glutamic acid	36	[596; N-Acetylglutamic acid (2TMS)]	60	0.260	0.599	13.358	0.508	42	99	32	109	8	32 duplicate
5002	42	Glutamic acid	124	[734; 1-Monooleoylglycerol (2TMS); 1-Monoheptadecenoylethanol (1TMS)]	55	0.255	0.437	44.805	0.356	43	98	41	100	140	117 original
4985	42	Glutamic acid	107	9-(Z)-Octadecenoic acid	60	0.241	0.311	19.564	0.378	44	97	49	92	26	106 original
4921	42	Glutamic acid	43	[546; Leucine (2TBS)]	57	0.231	0.309	25.660	0.390	45	96	50	91	60	100 original
5008	42	Glutamic acid	130	Trehalose	59	0.223	0.383	15.685	0.333	46	95	48	95	18	127 original
4897	42	Glutamic acid	119	[931; myo-Inositol-2-phosphate (7TMS)]	60	0.217	0.169	26.802	0.401	47	94	54	87	65	93 original
4949	42	Glutamic acid	71	[731; Erythrose (3TMS)]	60	0.195	0.368	21.066	0.431	48	93	48	93	33	79 original
5015	42	Glutamic acid	137	Ergosterol	60	0.186	0.373	21.388	0.369	49	92	47	94	34	112 original
4941	42	Glutamic acid	63	Glutamine	48	0.156	0.457	27.138	0.428	50	91	40	101	71	81 original
4968	42	Glutamic acid	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	60	0.121	0.013	26.914	0.334	51	90	57	84	68	124 original
10398	42	Glutamic acid	4	Phosphoric acid	49	0.121	0.551	11.901	0.500	52	89	36	105	7	38 duplicate
5016	42	Glutamic acid	138	[674; Ergosterol (1TMS)]	42	0.106	0.215	34.115	0.306	53	88	53	88	108	134 original
4972	42	Glutamic acid	94	Hexadecanoic acid	60	0.080	-0.004	19.089	0.335	54	87	58	83	23	123 original
5019	42	Glutamic acid	141	Lanosta-8,24-dien-3-beta-ol	57	0.063	-0.017	38.031	0.406	55	86	60	81	129	91 original
5017	42	Glutamic acid	139	[700; Ergosta-5,7-dien-3-ol]	35	0.062	0.113	34.442	0.280	56	85	55	86	109	135 original
4987	42	Glutamic acid	109	Octadecanoic acid	60	0.032	-0.084	22.506	0.314	57	84	63	78	41	133 original
4989	42	Glutamic acid	111	[583; Erythritol (4TMS)]	39	0.026	0.062	35.425	0.224	58	83	56	85	117	138 original
4931	42	Glutamic acid	53	Glycerol-2-phosphate	60	0.020	-0.127	35.369	0.333	59	82	64	77	116	126 original
5011	42	Glutamic acid	133	[855; Squalene]	60	0.002	0.286	26.991	0.374	60	81	52	89	70	110 original

4950	42	Glutamic acid	72	[918; D-Xylopyranose (4TMS)]	60	-0.008	-0.010	31.731	0.314	61	80	59	82	98	132	original
11839	42	Glutamic acid	15	Alanine	40	-0.050	-0.083	20.077	0.492	62	79	62	79	28	47	duplicate
5018	42	Glutamic acid	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	45	-0.061	-0.167	37.361	0.432	63	78	67	74	126	78	original
4971	42	Glutamic acid	93	[607; Putrescine (4TMS)]	56	-0.062	-0.439	40.124	0.418	64	77	84	57	131	88	original
4942	42	Glutamic acid	64	[789; Tyramine (3TMS)]	59	-0.074	-0.071	28.839	0.342	65	76	61	80	79	121	original
4957	42	Glutamic acid	79	Glucose	60	-0.118	-0.269	21.465	0.423	66	75	71	70	35	83	original
4962	42	Glutamic acid	84	Mannitol	58	-0.129	-0.711	24.705	0.501	67	74	113	28	64	35	original
4996	42	Glutamic acid	118	[928; Glucopyranose-6-phosphate (6TMS)]	54	-0.129	-0.130	28.604	0.341	68	73	65	76	83	122	original
4961	42	Glutamic acid	83	Sorbitol	55	-0.149	0.412	14.432	0.498	69	72	43	98	12	40	original
5005	42	Glutamic acid	127	[777; Fructose-6-phosphate methoxamine (6TMS)]	35	-0.200	-0.436	18.442	0.185	70	71	81	60	21	140	original
4994	42	Glutamic acid	116	[882; Pseudouridine (5TMS)]	29	-0.227	-0.298	25.310	0.360	71	70	73	68	59	115	original
5001	42	Glutamic acid	123	[945; Galactofuranose-6-phosphate (7TMS)]	60	-0.231	-0.154	23.598	0.438	72	69	66	75	47	73	original
4974	42	Glutamic acid	86	myo-Inositol	47	-0.232	-0.184	41.423	0.325	73	68	68	73	135	128	original
4952	42	Glutamic acid	74	[912; Tetradecanoic acid (1TMS)]	60	-0.252	-0.343	33.204	0.455	74	67	76	65	104	69	original
4925	42	Glutamic acid	47	[NA]	60	-0.253	-0.361	31.533	0.384	75	66	77	64	98	103	original
5004	42	Glutamic acid	128	[559; Erythritol (4TMS)]	41	-0.266	-0.253	23.473	0.391	76	65	70	71	44	99	original
4963	42	Glutamic acid	85	[529; Methylcitric acid (4TMS)]	47	-0.269	-0.571	28.619	0.580	77	64	95	46	76	10	original
5013	42	Glutamic acid	135	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	60	-0.273	-0.439	22.077	0.398	78	63	83	58	38	95	original
4992	42	Glutamic acid	114	Fructose-6-phosphate	49	-0.286	-0.389	28.810	0.330	79	62	79	62	86	128	original
4982	42	Glutamic acid	104	[795; Erythritol (4TMS)]	60	-0.289	-0.276	29.742	0.414	80	61	72	69	84	90	original
14764	42	Glutamic acid	41	[639; Proline (2TMS)]	60	-0.329	-0.219	22.256	0.347	81	60	69	72	39	120	duplicate
5010	42	Glutamic acid	132	[895; Isomaltose methoxamine (8TMS)]	38	-0.334	-0.658	32.261	0.317	82	59	107	34	100	131	original
4990	42	Glutamic acid	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	59	-0.340	-0.490	40.659	0.395	83	58	88	53	134	96	original
4980	42	Glutamic acid	102	[904; Galactose methoxamine (5TMS)]	60	-0.344	-0.479	31.504	0.439	84	57	86	55	95	72	original
4991	42	Glutamic acid	113	Galactose-6-phosphate	58	-0.355	-0.430	32.952	0.377	85	56	80	61	103	108	original
12211	42	Glutamic acid	18	[590; 1-Acetyl-2-thiohydantoin]	60	-0.360	-0.385	26.887	0.351	86	55	78	63	67	118	duplicate
5006	42	Glutamic acid	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	41	-0.360	-0.592	21.587	0.253	87	54	99	42	36	138	original
12333	42	Glutamic acid	19	Alanine (BP) (3TMS)	60	-0.398	-0.337	24.945	0.394	88	52	75	66	56	97	duplicate
4978	42	Glutamic acid	100	[857; Mannitol (6TMS)]	60	-0.398	-0.602	26.265	0.433	89	53	100	41	64	77	original
4998	42	Glutamic acid	120	[945; Uridine (3TMS)]	50	-0.409	-0.438	21.026	0.467	90	51	82	59	32	62	original
10669	42	Glutamic acid	6	Glycerol	60	-0.415	-0.483	23.908	0.384	91	50	87	54	50	104	duplicate
9984	42	Glutamic acid	1	[938; Sulfuric acid (2TMS)]	32	-0.444	-0.661	20.107	0.228	92	49	108	33	29	137	duplicate
4958	42	Glutamic acid	80	[772; D-Glucose (5TMS)]	58	-0.445	-0.473	23.815	0.379	93	48	85	56	49	105	original
4922	42	Glutamic acid	44	[910; 2-Ketogluconic acid methoxamine (4TMS)]	46	-0.447	-0.495	25.001	0.333	94	47	89	52	58	125	original
4969	42	Glutamic acid	91	[766; beta-D-Methylglucopyranoside (4TMS)]	60	-0.477	-0.697	35.924	0.455	95	46	111	30	121	68	original
11456	42	Glutamic acid	12	Glyceric acid	59	-0.495	-0.770	36.567	0.472	96	45	124	17	124	58	duplicate
4975	42	Glutamic acid	97	[756; beta-D-Methylglucopyranoside (4TMS)]	48	-0.498	-0.709	27.518	0.416	97	44	112	29	73	88	original
14149	42	Glutamic acid	35	Pyroglutamic acid	60	-0.498	-0.585	24.411	0.458	98	43	98	43	51	67	duplicate
4999	42	Glutamic acid	121	[657; Erythritol (4TMS)]	51	-0.506	-0.507	35.487	0.350	99	42	90	51	118	119	original
13386	42	Glutamic acid	28	Malic acid	60	-0.507	-0.724	25.930	0.510	100	41	114	27	62	31	duplicate
4988	42	Glutamic acid	110	[715; Erythritol (4TMS)]	50	-0.510	-0.560	32.468	0.438	101	40	92	49	102	74	original
13159	42	Glutamic acid	26	Citramalic acid	60	-0.511	-0.623	19.953	0.440	102	39	105	38	27	71	duplicate
4993	42	Glutamic acid	115	Glucose-6-phosphate	58	-0.514	-0.566	20.932	0.425	103	38	93	48	31	82	original
5000	42	Glutamic acid	122	[644; Erythritol (4TMS)]	48	-0.521	-0.609	35.861	0.389	104	37	103	38	120	101	original
4995	42	Glutamic acid	117	[724; Glycerol (3TMS)]	52	-0.525	-0.574	30.205	0.385	105	36	97	44	89	102	original
12574	42	Glutamic acid	21	[678; N,N-Di(2-Hydroxyethyl)-methanamine (2TMS)]	60	-0.542	-0.695	21.724	0.484	106	35	110	31	37	51	duplicate
5003	42	Glutamic acid	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	60	-0.542	-0.573	24.531	0.404	107	34	98	45	53	92	original
4985	42	Glutamic acid	87	[945; beta-D-Glucopyranose (5TMS)]	59	-0.550	-0.558	26.076	0.378	108	33	91	50	63	107	original
4954	42	Glutamic acid	76	Fructose	60	-0.553	-0.619	24.971	0.429	109	32	104	37	57	80	original
12693	42	Glutamic acid	22	[690; N,N-Di(2-Hydroxyethyl)-methanamine (2TMS)]	50	-0.554	-0.727	35.577	0.480	110	31	115	28	119	48	duplicate



4983	42	Glutamic acid	105	[705; 2-Ketogluconic acid (5TMS)]	44	-0.564	-0.777	25.820	0.368	111	30	126	15	61	113 original
14684	42	Glutamic acid	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	60	-0.566	-0.666	19.248	0.480	112	29	109	32	24	64 duplicate
11713	42	Glutamic acid	14	Fumaric acid	60	-0.569	-0.755	34.891	0.503	113	28	118	23	114	34 duplicate
4956	42	Glutamic acid	78	Mannose	58	-0.584	-0.604	36.070	0.375	114	27	101	40	123	108 original
4979	42	Glutamic acid	101	[832; Dopamine (4TMS)]	60	-0.584	-0.737	32.175	0.470	115	26	117	24	99	80 original
4970	42	Glutamic acid	92	[680; Glycero-2-phosphate (4TMS)]	50	-0.585	-0.567	28.647	0.324	116	25	94	47	77	130 original
4977	42	Glutamic acid	99	[682; Ribose-5-phosphate methoxamine (BP) (5TMS)]	37	-0.589	-0.781	26.882	0.359	117	24	127	14	66	116 original
4948	42	Glutamic acid	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	54	-0.600	-0.321	20.321	0.369	118	23	74	67	30	111 original
4984	42	Glutamic acid	106	[733; Threitol (4TMS)]	58	-0.608	-0.653	30.846	0.472	119	22	106	35	92	59 original
4981	42	Glutamic acid	103	[648; Ethylamine (2TMS)]	59	-0.615	-0.767	33.370	0.480	120	21	123	18	105	53 original
11329	42	Glutamic acid	11	Succinic acid	60	-0.617	-0.733	27.616	0.475	121	20	116	25	74	57 duplicate
4951	42	Glutamic acid	73	[708; Glucose methoxamine (5TMS)]	54	-0.627	-0.607	34.766	0.466	122	19	102	39	113	63 original
4932	42	Glutamic acid	54	[NA]	51	-0.633	-0.760	34.717	0.417	123	18	120	21	112	87 original
14461	42	Glutamic acid	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	60	-0.647	-0.812	28.727	0.501	124	17	133	8	78	38 duplicate
13498	42	Glutamic acid	29	Erythritol	-60	-0.655	-0.837	30.422	0.537	125	16	136	5	90	22 duplicate
5012	42	Glutamic acid	134	Isomaltose	60	-0.685	-0.817	28.200	0.489	126	15	134	7	81	49 original
12088	42	Glutamic acid	17	[700; 2-methyl-1,2-propanediol (2TMS)]	60	-0.690	-0.795	24.936	0.496	127	14	128	13	55	42 duplicate
4940	42	Glutamic acid	62	[812; D-Xylofuranose (4TMS)]	60	-0.692	-0.758	22.859	0.476	128	13	119	22	42	58 original
4934	42	Glutamic acid	56	[828; Orolic acid (3TMS)]	60	-0.694	-0.810	37.440	0.498	129	12	131	10	127	41 original
4935	42	Glutamic acid	57	[757; 2-Desoxy-pentos-3-yose dimethoxamine (2TMS)]	51	-0.700	-0.764	30.889	0.419	130	11	122	19	93	84 original
4966	42	Glutamic acid	88	Gluconic acid	60	-0.707	-0.775	30.014	0.531	131	10	125	16	88	25 original
14563	42	Glutamic acid	39	[829; 1-Phenylethanol (1TMS)]	59	-0.719	-0.836	30.985	0.483	132	9	135	6	94	52 duplicate
4964	42	Glutamic acid	86	[793; D-Galactono-1,4-lactone (4TMS)]	58	-0.725	-0.764	34.641	0.493	133	8	121	20	110	46 original
11586	42	Glutamic acid	13	Uracil	60	-0.727	-0.860	26.927	0.527	134	7	138	3	89	28 duplicate
5007	42	Glutamic acid	129	[840; Maltose methoxamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	55	-0.732	-0.805	33.962	0.437	135	6	130	11	107	75 original
12928	42	Glutamic acid	24	[725; 2-Ketocanoic acid (2TMS)]	60	-0.733	-0.850	23.534	0.528	136	5	137	4	46	27 duplicate
4943	42	Glutamic acid	65	[646; 3-Deoxyglucitol (5TMS)]	59	-0.735	-0.810	38.780	0.478	137	4	132	9	130	55 original
11964	42	Glutamic acid	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	60	-0.737	-0.868	23.783	0.532	138	3	140	1	48	24 duplicate
4924	42	Glutamic acid	46	Arabinose	60	-0.741	-0.789	33.478	0.485	139	2	129	12	106	50 original
4928	42	Glutamic acid	50	[746; Ribonic acid-1,4-lactone (3TMS)]	57	-0.768	-0.865	43.218	0.516	140	1	139	2	137	30 original
13045	43	[548; Leucine (2TBS)]	25	[709; 2,5-Diaminovalerolactam (2TMS)]	44	0.545	0.692	11.903	0.396	1	140	1	140	46	84 duplicate
13274	43	[548; Leucine (2TBS)]	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	51	0.449	0.561	16.689	0.427	2	139	7	134	91	61 duplicate
12812	43	[548; Leucine (2TBS)]	23	Homoserine	60	0.417	0.628	6.864	0.460	3	138	3	138	5	41 duplicate
5021	43	[548; Leucine (2TBS)]	45	Homocysteine	58	0.393	0.591	21.385	0.450	4	137	6	135	114	47 original
5044	43	[548; Leucine (2TBS)]	68	[570; Hypoxanthine (2TMS)]	19	0.392	0.636	13.828	0.566	5	136	2	139	61	3 original
13720	43	[548; Leucine (2TBS)]	31	[622; Parabanic acid (2TMS)]	60	0.356	0.492	10.475	0.393	6	135	10	131	32	87 duplicate
5024	43	[548; Leucine (2TBS)]	48	Asparagine	60	0.350	0.539	8.569	0.514	7	134	8	133	20	9 original
13937	43	[548; Leucine (2TBS)]	33	Methionine	60	0.339	0.455	7.599	0.461	8	133	15	126	9	39 duplicate
5045	43	[548; Leucine (2TBS)]	69	Arginine	57	0.333	0.537	16.616	0.480	9	132	9	132	90	25 original
5058	43	[548; Leucine (2TBS)]	82	Lysine	38	0.331	0.626	13.066	0.571	10	131	4	137	56	2 original
5025	43	[548; Leucine (2TBS)]	49	[877; Pyrophosphoric acid (4TMS)]	60	0.329	0.472	18.811	0.421	11	130	12	129	103	66 original
5035	43	[548; Leucine (2TBS)]	59	Omitine; Arginine	60	0.325	0.406	36.010	0.396	12	129	19	122	138	85 original
10124	43	[548; Leucine (2TBS)]	2	Serine	59	0.324	0.242	15.776	0.389	13	128	28	113	79	93 duplicate
13829	43	[548; Leucine (2TBS)]	32	[729; N,N-Dimethyllysine methyl ester]	59	0.316	0.399	13.773	0.458	14	127	20	121	59	42 duplicate
10937	43	[548; Leucine (2TBS)]	8	Isoleucine	52	0.306	0.200	15.415	0.345	15	126	35	106	78	125 duplicate
5074	43	[548; Leucine (2TBS)]	98	[697; Ribose-5-phosphate methoxamine (5TMS)]	45	0.305	0.460	18.277	0.415	16	125	14	127	100	73 original
13610	43	[548; Leucine (2TBS)]	30	[815; Ethyl-3(2H)-thiophanone]	60	0.302	0.412	25.428	0.415	17	124	18	123	123	71 duplicate
5107	43	[548; Leucine (2TBS)]	131	[626; 5-Methylthioadenosine (3TMS)]	52	0.300	0.489	16.408	0.499	18	123	11	130	87	14 original
14044	43	[548; Leucine (2TBS)]	34	Aspartic acid	60	0.285	0.413	28.272	0.445	19	122	17	124	131	50 duplicate

10535	43 [548; Leucine (2TBS)]	5	Leucine	44	0.281	0.597	8.236	0.451	20	121	5	136	16	46 duplicate
11069	43 [548; Leucine (2TBS)]	9	Proline	60	0.273	0.234	23.712	0.387	21	120	29	112	120	96 duplicate
11200	43 [548; Leucine (2TBS)]	10	Glycine	60	0.272	0.464	14.405	0.488	22	119	13	128	85	21 duplicate
5039	43 [548; Leucine (2TBS)]	63	Glutamine	48	0.262	0.196	14.754	0.488	23	118	37	104	69	22 original
5042	43 [548; Leucine (2TBS)]	66	Glycetic acid-3-phosphate	60	0.246	0.250	7.148	0.383	24	117	25	116	6	89 original
5065	43 [548; Leucine (2TBS)]	89	[775; Dopamine (4TMS)]	34	0.244	0.367	15.146	0.540	25	116	21	120	76	6 original
5053	43 [548; Leucine (2TBS)]	77	[826; beta-[(5-methyl-2-thienyl)methyl]amino-benzeneacetic acid methyl ester]	58	0.240	0.311	25.497	0.421	26	115	22	119	124	67 original
5051	43 [548; Leucine (2TBS)]	75	Lysine	60	0.232	0.200	34.762	0.375	27	114	34	107	137	105 original
14864	43 [548; Leucine (2TBS)]	42	Glutamic acid	57	0.231	0.309	25.660	0.390	28	113	23	118	126	90 duplicate
5027	43 [548; Leucine (2TBS)]	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	0.230	0.448	20.601	0.430	29	112	16	125	110	59 original
5034	43 [548; Leucine (2TBS)]	58	[636; 4R-Acetimido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	60	0.206	0.197	11.954	0.381	30	111	36	105	47	101 original
5057	43 [548; Leucine (2TBS)]	81	Tyrosine	60	0.190	0.221	29.877	0.508	31	110	30	111	134	12 original
5037	43 [548; Leucine (2TBS)]	61	(NA)	60	0.176	0.143	6.003	0.391	32	109	41	100	2	89 original
10262	43 [548; Leucine (2TBS)]	3	Ethanolamine	58	0.160	0.252	11.383	0.493	33	108	24	117	41	15 duplicate
9885	43 [548; Leucine (2TBS)]	1	[938; Sulfuric acid (2TMS)]	32	0.141	0.047	8.377	0.351	34	107	49	92	19	121 duplicate
14359	43 [548; Leucine (2TBS)]	37	Phenylalanine	60	0.130	0.207	18.266	0.368	35	108	32	109	99	115 duplicate
5023	43 [548; Leucine (2TBS)]	47	(NA)	60	0.122	0.152	10.380	0.371	36	105	40	101	30	112 original
14255	43 [548; Leucine (2TBS)]	36	[596; N-Acetylglutamic acid (2TMS)]	60	0.120	0.040	24.096	0.350	37	104	50	91	121	123 duplicate
10389	43 [548; Leucine (2TBS)]	4	Phosphoric acid	48	0.105	0.082	28.835	0.284	38	103	47	94	132	138 duplicate
5087	43 [548; Leucine (2TBS)]	91	[766; beta-D-Methylglucopyranoside (4TMS)]	60	0.103	0.102	15.974	0.441	39	102	44	97	83	53 original
5084	43 [548; Leucine (2TBS)]	108	Octadecenoic acid	60	0.097	0.082	8.216	0.359	40	101	46	95	15	118 original
10804	43 [548; Leucine (2TBS)]	7	Threonine	60	0.090	0.157	25.524	0.389	41	100	38	103	125	92 duplicate
5031	43 [548; Leucine (2TBS)]	55	[612; 4-Aminobutyric acid (2TBS)]	42	0.087	0.135	22.706	0.464	42	99	42	99	118	36 original
11840	43 [548; Leucine (2TBS)]	15	Alanine	60	0.085	0.156	14.557	0.491	43	98	39	102	66	18 duplicate
5071	43 [548; Leucine (2TBS)]	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	48	0.080	0.202	21.127	0.543	44	97	33	108	113	5 original
5112	43 [548; Leucine (2TBS)]	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	15	0.067	0.244	3.887	0.150	45	96	28	115	1	140 original
5106	43 [548; Leucine (2TBS)]	130	Trehalose	59	0.053	0.056	25.189	0.336	46	95	48	93	122	129 original
5029	43 [548; Leucine (2TBS)]	53	Glycerol-2-phosphate	60	0.047	0.207	11.658	0.353	47	94	31	110	45	119 original
5069	43 [548; Leucine (2TBS)]	93	[607; Putrescine (4TMS)]	57	0.041	0.128	17.353	0.337	48	93	43	98	93	128 original
5073	43 [548; Leucine (2TBS)]	97	[756; beta-D-Methylglucopyranoside (4TMS)]	48	0.039	-0.016	18.425	0.369	49	92	53	88	101	114 original
5048	43 [548; Leucine (2TBS)]	72	[919; D-Xylopyranose (4TMS)]	59	0.036	-0.009	10.336	0.385	50	91	52	89	29	97 original
5028	43 [548; Leucine (2TBS)]	52	(NA)	42	0.031	0.020	19.379	0.556	51	90	51	90	108	4 original
5040	43 [548; Leucine (2TBS)]	64	[769; Tyramine (3TMS)]	59	0.018	0.088	6.406	0.352	52	89	45	96	3	120 original
5094	43 [548; Leucine (2TBS)]	118	[828; Glucopyranose-6-phosphate (6TMS)]	54	-0.008	-0.071	10.426	0.325	53	88	60	81	31	133 original
5077	43 [548; Leucine (2TBS)]	101	[832; Dopamine (4TMS)]	60	-0.021	-0.033	10.697	0.436	54	86	55	86	33	55 original
5043	43 [548; Leucine (2TBS)]	67	Citric acid	60	-0.021	-0.035	19.350	0.389	55	87	56	85	107	81 original
5056	43 [548; Leucine (2TBS)]	80	[772; D-Glucose (5TMS)]	59	-0.027	-0.127	26.829	0.385	56	85	84	77	127	88 original
5036	43 [548; Leucine (2TBS)]	60	Glycerol-3-phosphate	60	-0.034	-0.059	17.399	0.456	57	84	59	82	94	43 original
5055	43 [548; Leucine (2TBS)]	79	Glucose	60	-0.035	-0.086	30.344	0.476	58	83	61	80	135	30 original
12455	43 [548; Leucine (2TBS)]	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.037	0.242	16.090	0.618	59	82	27	114	85	1 duplicate
5115	43 [548; Leucine (2TBS)]	139	[700; Ergosta-5,7-dien-3-ol]	35	-0.039	-0.038	16.525	0.343	60	81	57	84	89	127 original
5060	43 [548; Leucine (2TBS)]	84	Mannitol	59	-0.039	-0.028	27.080	0.387	61	80	54	87	128	95 original
5079	43 [548; Leucine (2TBS)]	103	[648; Ethylamine (2TMS)]	59	-0.059	-0.099	14.170	0.429	62	79	62	79	63	60 original
5081	43 [548; Leucine (2TBS)]	105	[705; 2-Ketogluconic acid (5TMS)]	44	-0.085	-0.204	12.438	0.344	63	78	69	72	52	128 original
5066	43 [548; Leucine (2TBS)]	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	60	-0.088	-0.213	7.261	0.374	64	77	71	70	7	108 original
5083	43 [548; Leucine (2TBS)]	107	9-(Z)-Octadecenoic acid	60	-0.089	-0.143	10.989	0.363	65	76	65	76	38	117 original
5063	43 [548; Leucine (2TBS)]	87	[945; beta-D-Glucopyranose (5TMS)]	58	-0.108	-0.217	30.985	0.371	66	75	72	69	136	110 original
5075	43 [548; Leucine (2TBS)]	89	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	37	-0.111	-0.361	12.016	0.404	67	74	90	51	48	78 original

5110	43 [548; Leucine (2TBS)]	134 Isomaltose	60 -0.123	-0.379	22.645	0.491	68	73	98	43	117	17 original
5098	43 [548; Leucine (2TBS)]	123 [945; Galactofuranose-6-phosphate (7TMS)]	60 -0.130	-0.198	8.335	0.476	69	72	68	73	18	31 original
5088	43 [548; Leucine (2TBS)]	92 [680; Glycerol-2-phosphate (4TMS)]	50 -0.135	-0.155	10.981	0.290	70	71	66	75	37	137 original
5100	43 [548; Leucine (2TBS)]	124 [734; 1-Monoleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]	55 -0.138	-0.107	23.323	0.378	71	70	63	78	119	103 original
5041	43 [548; Leucine (2TBS)]	65 [846; 3-Deoxyglucitol (5TMS)]	59 -0.149	-0.394	17.489	0.508	72	69	101	40	96	13 original
5059	43 [548; Leucine (2TBS)]	83 Sorbitol	54 -0.159	-0.049	17.327	0.335	73	68	58	83	92	130 original
5095	43 [548; Leucine (2TBS)]	119 [931; myo-Inositol-2-phosphate (7TMS)]	60 -0.159	-0.304	8.865	0.375	74	67	81	60	25	104 original
5047	43 [548; Leucine (2TBS)]	71 [731; Erythrose (3TMS)]	60 -0.163	-0.247	8.823	0.372	75	68	73	68	21	109 original
10870	43 [548; Leucine (2TBS)]	6 Glycerol	60 -0.168	-0.179	36.628	0.422	76	65	67	74	140	65 duplicate
5032	43 [548; Leucine (2TBS)]	56 [828; Orolic acid (3TMS)]	60 -0.176	-0.363	15.020	0.489	77	64	91	50	73	19 original
5033	43 [548; Leucine (2TBS)]	57 [757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	51 -0.176	-0.379	15.961	0.399	78	63	97	44	82	80 original
11587	43 [548; Leucine (2TBS)]	13 Ureol	60 -0.181	-0.409	14.343	0.479	79	62	103	38	64	27 duplicate
5109	43 [548; Leucine (2TBS)]	133 [855; Squalene]	60 -0.182	-0.270	8.809	0.347	80	61	76	65	23	124 original
5103	43 [548; Leucine (2TBS)]	127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	35 -0.187	-0.251	7.619	0.299	81	60	74	67	10	138 original
12089	43 [548; Leucine (2TBS)]	17 [700; 2-methyl-1,2-propanediol (2TMS)]	60 -0.193	-0.356	14.942	0.414	82	59	88	53	71	74 duplicate
5022	43 [548; Leucine (2TBS)]	46 Arabinose	60 -0.201	-0.365	18.028	0.512	83	58	92	49	98	10 original
5030	43 [548; Leucine (2TBS)]	54 [NA]	51 -0.202	-0.355	15.077	0.351	84	57	87	54	74	122 original
5080	43 [548; Leucine (2TBS)]	104 [785; Erythritol (4TMS)]	59 -0.202	-0.337	9.422	0.524	85	56	84	57	26	7 original
11965	43 [548; Leucine (2TBS)]	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	60 -0.203	-0.414	14.703	0.466	86	55	105	38	68	35 duplicate
5062	43 [548; Leucine (2TBS)]	86 [783; D-Galactono-1,4-lactone (4TMS)]	58 -0.204	-0.365	22.293	0.464	87	54	93	48	115	37 original
12929	43 [548; Leucine (2TBS)]	24 [725; 2-Ketocanolic acid (2TMS)]	60 -0.205	-0.422	27.707	0.509	88	53	108	33	129	11 duplicate
5105	43 [548; Leucine (2TBS)]	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-O-Glc]	55 -0.205	-0.411	14.960	0.455	89	52	104	37	72	44 original
5064	43 [548; Leucine (2TBS)]	88 Gluconic acid	60 -0.208	-0.375	12.447	0.487	90	51	94	47	53	23 original
5089	43 [548; Leucine (2TBS)]	113 Galactose-6-phosphate	58 -0.214	-0.264	11.489	0.478	91	50	75	66	44	28 original
14765	43 [548; Leucine (2TBS)]	41 [639; Proline (2TMS)]	60 -0.214	-0.382	11.188	0.435	92	49	100	41	40	56 duplicate
5049	43 [548; Leucine (2TBS)]	73 [708; Glucose methoxyamine (5TMS)]	53 -0.218	-0.421	13.800	0.481	93	48	107	34	60	24 original
5072	43 [548; Leucine (2TBS)]	98 myo-Inositol	47 -0.227	-0.271	18.195	0.335	94	47	77	64	106	131 original
5038	43 [548; Leucine (2TBS)]	62 [812; D-Xylofuranose (4TMS)]	60 -0.228	-0.378	10.906	0.463	95	46	95	46	38	38 original
5104	43 [548; Leucine (2TBS)]	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	41 -0.232	-0.297	9.720	0.278	96	45	80	61	27	139 original
14564	43 [548; Leucine (2TBS)]	39 [828; 1-Phenylethanol (1TMS)]	59 -0.233	-0.458	16.380	0.468	97	44	111	30	86	34 duplicate
5046	43 [548; Leucine (2TBS)]	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	53 -0.253	-0.291	15.095	0.373	98	43	79	62	75	108 original
14462	43 [548; Leucine (2TBS)]	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	60 -0.255	-0.491	8.318	0.435	99	42	120	21	17	57 duplicate
5113	43 [548; Leucine (2TBS)]	137 Ergosterol	60 -0.258	-0.342	12.286	0.398	100	40	85	56	50	94 original
12334	43 [548; Leucine (2TBS)]	19 Alanine (BP) (3TMS)	60 -0.258	-0.380	10.715	0.442	101	41	99	42	34	51 duplicate
5028	43 [548; Leucine (2TBS)]	50 [748; Ribonic acid-1,4-lactone (3TMS)]	57 -0.264	-0.451	20.513	0.416	102	39	109	32	109	70 original
5116	43 [548; Leucine (2TBS)]	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	46 -0.266	-0.419	15.878	0.383	103	38	106	35	81	100 original
13499	43 [548; Leucine (2TBS)]	29 Erythritol	60 -0.267	-0.453	7.638	0.449	104	37	110	31	11	49 duplicate
5090	43 [548; Leucine (2TBS)]	114 Fructose-6-phosphate	49 -0.269	-0.344	11.173	0.480	105	36	86	55	39	26 original
11330	43 [548; Leucine (2TBS)]	11 Succinic acid	60 -0.270	-0.405	7.382	0.410	106	35	102	39	8	75 duplicate
5117	43 [548; Leucine (2TBS)]	141 Lanosta-8,24-dien-3-beta-ol	58 -0.286	-0.459	16.014	0.371	107	34	112	29	84	111 original
5096	43 [548; Leucine (2TBS)]	120 [945; Uridine (3TMS)]	50 -0.300	-0.208	9.843	0.398	108	33	70	71	28	82 original
5087	43 [548; Leucine (2TBS)]	111 [583; Erythritol (2TMS)]	39 -0.304	-0.318	19.165	0.329	109	32	82	59	105	132 original
12694	43 [548; Leucine (2TBS)]	22 [690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	50 -0.304	-0.490	14.817	0.434	110	31	119	22	70	58 duplicate
11459	43 [548; Leucine (2TBS)]	12 Glycic acid	59 -0.314	-0.475	13.246	0.392	111	30	116	25	58	88 duplicate
5054	43 [548; Leucine (2TBS)]	78 Mannose	58 -0.316	-0.463	14.572	0.488	112	29	113	28	67	20 original
5114	43 [548; Leucine (2TBS)]	138 [674; Ergosterol (1TMS)]	42 -0.319	-0.472	15.363	0.481	113	28	115	26	77	40 original
5101	43 [548; Leucine (2TBS)]	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	60 -0.321	-0.278	28.024	0.454	114	27	78	63	130	45 original
5085	43 [548; Leucine (2TBS)]	109 Octadecanoic acid	60 -0.323	-0.588	20.807	0.438	115	26	135	6	111	54 original

11714	43 [548; Leucine (2TBS)]	14	Fumaric acid	60	-0.327	-0.508	11.398	0.425	116	25	122	19	42	62 duplicate
5091	43 [548; Leucine (2TBS)]	115	Glucose-6-phosphate	58	-0.327	-0.330	21.028	0.405	117	24	83	58	112	77 original
5091	43 [548; Leucine (2TBS)]	85	[529; Methylenic acid (4TMS)]	46	-0.328	-0.534	6.759	0.424	118	23	128	13	4	64 original
12575	43 [548; Leucine (2TBS)]	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	60	-0.333	-0.530	13.225	0.415	119	22	128	15	57	72 duplicate
13367	43 [548; Leucine (2TBS)]	28	Malic acid	60	-0.337	-0.551	7.882	0.477	120	21	129	12	14	29 duplicate
12212	43 [548; Leucine (2TBS)]	18	[590; 1-Acetyl-2-thiohydantoin]	60	-0.338	-0.533	7.670	0.408	121	20	127	14	12	76 duplicate
13160	43 [548; Leucine (2TBS)]	26	Citramalic acid	60	-0.344	-0.525	12.386	0.420	122	19	125	16	51	68 duplicate
5070	43 [548; Leucine (2TBS)]	94	Hexadecanoic acid	60	-0.353	-0.588	19.096	0.442	123	18	134	7	104	52 original
14150	43 [548; Leucine (2TBS)]	35	Pyroglutamic acid	60	-0.354	-0.359	36.397	0.492	124	17	89	52	139	16 duplicate
5052	43 [548; Leucine (2TBS)]	76	Fructose	60	-0.360	-0.379	22.433	0.472	125	15	96	45	116	33 original
5111	43 [548; Leucine (2TBS)]	135		60	-0.360	-0.483	8.779	0.378	126	16	118	23	22	102 original
5098	43 [548; Leucine (2TBS)]	112	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	59	-0.377	-0.469	17.475	0.395	127	14	114	27	95	88 original
5082	43 [548; Leucine (2TBS)]	106	[877; beta-D-Galactopyranoside-(1,2)-glycerol (8TMS)]	58	-0.379	-0.505	12.750	0.519	128	13	121	20	54	8 original
14665	43 [548; Leucine (2TBS)]	40	[733; Threitol (4TMS)]	60	-0.403	-0.566	29.618	0.476	129	12	131	10	133	32 duplicate
5093	43 [548; Leucine (2TBS)]	117	[724; Glycerol (3TMS)]	52	-0.410	-0.584	12.258	0.397	130	11	133	8	49	83 original
5108	43 [548; Leucine (2TBS)]	132	[895; Isomaltose methoxamine (8TMS)]	38	-0.425	-0.557	17.894	0.312	131	10	130	11	97	135 original
5078	43 [548; Leucine (2TBS)]	100	[857; Mannitol (6TMS)]	60	-0.436	-0.520	7.851	0.398	132	9	124	17	13	81 original
5086	43 [548; Leucine (2TBS)]	110	[715; Erythritol (4TMS)]	60	-0.441	-0.479	8.810	0.403	133	8	117	24	79	original
5097	43 [548; Leucine (2TBS)]	121	[657; Erythritol (4TMS)]	51	-0.465	-0.586	16.435	0.418	135	6	137	4	88	63 original
5050	43 [548; Leucine (2TBS)]	72	[644; Erythritol (4TMS)]	60	-0.489	-0.556	14.151	0.449	136	5	140	1	62	48 original
5098	43 [548; Leucine (2TBS)]	122	[644; Erythritol (4TMS)]	48	-0.496	-0.820	18.702	0.369	137	4	138	3	102	113 original
5092	43 [548; Leucine (2TBS)]	116	[882; Pseudouridine (5TMS)]	28	-0.508	-0.513	10.791	0.320	138	3	123	18	35	134 original
5020	43 [548; Leucine (2TBS)]	44	[910; 2-Ketogluconic acid methoxamine (4TMS)]	46	-0.515	-0.591	12.752	0.367	139	2	136	5	55	116 original
5102	43 [548; Leucine (2TBS)]	128	[559; Erythritol (4TMS)]	41	-0.546	-0.845	11.479	0.373	140	1	139	2	43	107 original
5183	44 [910; 2-Ketogluconic acid]	110	[715; Erythritol (4TMS)]	49	0.871	0.978	5.171	0.664	1	140	1	140	3	4 original
5190	44 [910; 2-Ketogluconic acid]	117	[724; Glycerol (3TMS)]	47	0.858	0.953	4.271	0.641	2	139	4	137	1	13 original
5195	44 [910; 2-Ketogluconic acid]	122	[644; Erythritol (4TMS)]	48	0.842	0.961	12.069	0.642	3	138	2	139	51	12 original
5179	44 [910; 2-Ketogluconic acid]	106	[733; Threitol (4TMS)]	48	0.835	0.957	4.817	0.698	4	137	3	138	2	1 original
5194	44 [910; 2-Ketogluconic acid]	121	[657; Erythritol (4TMS)]	47	0.796	0.918	11.980	0.650	5	136	6	135	50	8 original
5149	44 [910; 2-Ketogluconic acid]	76	Fructose	50	0.783	0.912	21.312	0.666	6	135	7	134	111	3 original
5189	44 [910; 2-Ketogluconic acid]	126	[559; Erythritol (4TMS)]	45	0.758	0.920	7.137	0.637	7	134	5	136	12	17 original
14666	44 [910; 2-Ketogluconic acid]	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	50	0.722	0.890	27.985	0.586	8	133	8	133	132	38 duplicate
5188	44 [910; 2-Ketogluconic acid]	115	Glucose-6-phosphate	49	0.643	0.827	20.461	0.639	9	132	9	132	107	16 original
5173	44 [910; 2-Ketogluconic acid]	100	[857; Mannitol (6TMS)]	50	0.613	0.795	7.559	0.530	10	131	14	127	14	72 original
5147	44 [910; 2-Ketogluconic acid]	74	[912; Tetradecanoic acid (1TMS)]	50	0.602	0.777	6.875	0.482	11	130	19	122	11	83 original
14151	44 [910; 2-Ketogluconic acid]	35	Pyroglutamic acid	50	0.580	0.789	35.048	0.580	12	129	16	125	139	42 duplicate
5151	44 [910; 2-Ketogluconic acid]	78	Mannose	48	0.568	0.806	6.399	0.636	13	128	12	129	6	18 original
13388	44 [910; 2-Ketogluconic acid]	28	Malic acid	50	0.543	0.801	8.241	0.539	14	127	13	128	20	64 duplicate
5146	44 [910; 2-Ketogluconic acid]	73	[708; Glucose methoxamine (5TMS)]	43	0.542	0.786	6.269	0.535	15	126	17	124	4	87 original
5175	44 [910; 2-Ketogluconic acid]	102	[904; Galactose methoxamine (5TMS)]	50	0.536	0.748	9.006	0.540	16	125	24	117	26	63 original
5208	44 [910; 2-Ketogluconic acid]	135		50	0.486	0.630	10.411	0.493	17	124	44	97	38	81 original
5159	44 [910; 2-Ketogluconic acid]	86	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	47	0.478	0.821	15.977	0.655	18	123	10	131	80	7 original
11715	44 [910; 2-Ketogluconic acid]	14	Fumaric acid	50	0.468	0.747	10.345	0.559	19	122	25	116	37	53 duplicate
14565	44 [910; 2-Ketogluconic acid]	39	[929; 1-Phenylethanol (1TMS)]	50	0.461	0.809	11.074	0.593	20	121	11	130	43	33 duplicate
14463	44 [910; 2-Ketogluconic acid]	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	50	0.460	0.792	7.156	0.646	21	120	15	126	13	10 duplicate
13161	44 [910; 2-Ketogluconic acid]	26	Citramalic acid	50	0.450	0.660	13.296	0.534	22	119	41	100	63	69 duplicate
12695	44 [910; 2-Ketogluconic acid]	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	42	0.449	0.741	10.203	0.607	23	118	27	114	34	28 duplicate
12576	44 [910; 2-Ketogluconic acid]	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	50	0.438	0.610	13.212	0.533	24	117	47	84	62	71 duplicate

5182	44 [910; 2-Ketogluconic acid 109	Octadecanoic acid	50	0.435	0.725	15.938	0.559	25	116	30	111	79	52 original
5167	44 [910; 2-Ketogluconic acid 94	Hexadecanoic acid	50	0.419	0.675	15.445	0.547	26	115	38	103	73	60 original
12213	44 [910; 2-Ketogluconic acid 18	[590; 1-Acetyl-2-biohydantoin]	50	0.416	0.550	8.376	0.463	27	114	53	88	22	93 duplicate
5185	44 [910; 2-Ketogluconic acid 112	[877; beta-D-Galactopyranoside-(1:2)-glycerol (6TMS)]	49	0.413	0.598	17.415	0.414	28	113	48	93	90	115 original
5158	44 [910; 2-Ketogluconic acid 85	[529; Methylcitric acid (4TMS)]	34	0.405	0.724	8.471	0.546	29	112	32	109	24	61 original
5213	44 [910; 2-Ketogluconic acid 140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	35	0.402	0.541	16.738	0.425	30	111	55	86	85	110 original
5205	44 [910; 2-Ketogluconic acid 132	[895; Isomaltose methoxyamine (6TMS)]	39	0.401	0.751	13.174	0.572	31	110	22	119	61	46 original
5214	44 [910; 2-Ketogluconic acid 141	[Lanosta-8,24-dien-3-beta-ol	47	0.397	0.560	14.833	0.453	32	109	51	90	69	96 original
11460	44 [910; 2-Ketogluconic acid 12	Glyceric acid	50	0.393	0.715	11.773	0.534	33	108	33	108	47	70 duplicate
13500	44 [910; 2-Ketogluconic acid 29	Erythritol	50	0.391	0.713	8.398	0.582	34	107	34	107	23	41 duplicate
5129	44 [910; 2-Ketogluconic acid 56	[829; Orolic acid (3TMS)]	50	0.388	0.744	6.628	0.629	35	106	26	115	7	23 original
5135	44 [910; 2-Ketogluconic acid 62	[812; D-Xylofuranose (4TMS)]	50	0.383	0.692	11.838	0.629	36	105	35	106	48	22 original
5161	44 [910; 2-Ketogluconic acid 88	Gluconic acid	50	0.373	0.618	9.490	0.614	37	104	46	95	27	27 original
5188	44 [910; 2-Ketogluconic acid 113	Galactose-6-phosphate	49	0.367	0.688	7.974	0.647	38	103	36	105	18	9 original
5193	44 [910; 2-Ketogluconic acid 120	[945; Uridine (3TMS)]	45	0.356	0.253	9.842	0.578	39	102	72	69	31	43 original
5119	44 [910; 2-Ketogluconic acid 46	Arabinose	50	0.355	0.755	12.455	0.633	40	101	21	120	56	19 original
12830	44 [910; 2-Ketogluconic acid 24	[725; 2-Ketocianonic acid (2TMS)]	50	0.353	0.749	26.838	0.640	41	100	23	118	129	14 duplicate
5143	44 [910; 2-Ketogluconic acid 70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	43	0.353	0.441	15.373	0.583	42	99	60	81	72	50 original
11966	44 [910; 2-Ketogluconic acid 16	[644; 2-Methyl-1,3-butanediol (2TMS)]	50	0.345	0.729	14.050	0.623	43	98	28	113	64	25 duplicate
5138	44 [910; 2-Ketogluconic acid 65	[646; 3-Deoxyglucitol (5TMS)]	50	0.344	0.765	6.395	0.632	44	97	18	123	5	20 original
5123	44 [910; 2-Ketogluconic acid 50	[746; Ribonic acid-1,4-lactone (3TMS)]	49	0.344	0.666	17.374	0.583	45	96	39	102	88	40 original
11588	44 [910; 2-Ketogluconic acid 13	Uracil	50	0.340	0.724	12.630	0.631	46	95	31	110	58	21 duplicate
5177	44 [910; 2-Ketogluconic acid 104	[795; Erythritol (4TMS)]	49	0.338	0.572	7.888	0.565	47	94	49	92	16	48 original
11331	44 [910; 2-Ketogluconic acid 11	Succinic acid	50	0.334	0.645	8.241	0.550	48	93	43	98	21	58 duplicate
5192	44 [910; 2-Ketogluconic acid 119	[831; myo-Inositol-2-phosphate (7TMS)]	50	0.332	0.325	9.538	0.442	49	92	69	72	28	102 original
5210	44 [910; 2-Ketogluconic acid 137	Ergosterol	50	0.331	0.303	11.455	0.446	50	91	70	71	44	101 original
5207	44 [910; 2-Ketogluconic acid 134	Isomaltose	50	0.321	0.761	20.741	0.655	51	90	20	121	109	6 original
5130	44 [910; 2-Ketogluconic acid 125	[757; 2-Desoxy-pentos-3-ylose dimethoxyamine (2TMS)]	49	0.310	0.727	8.051	0.639	52	89	29	112	19	15 original
5198	44 [910; 2-Ketogluconic acid 128	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	50	0.308	0.552	28.332	0.535	53	88	52	89	134	68 original
5201	44 [910; 2-Ketogluconic acid 105	[824; D-Sedoheptulose-7-phosphate (7TMS)]	44	0.307	0.563	6.845	0.537	54	87	50	91	10	66 original
5178	44 [910; 2-Ketogluconic acid 105	[705; 2-Ketogluconic acid (5TMS)]	48	0.294	0.495	10.134	0.543	55	86	58	83	33	62 original
12090	44 [910; 2-Ketogluconic acid 17	[700; 2-methyl-1,2-propanediol (2TMS)]	50	0.290	0.657	14.262	0.558	56	85	42	99	65	55 duplicate
5184	44 [910; 2-Ketogluconic acid 111	[583; Erythritol (4TMS)]	37	0.288	0.496	22.057	0.409	57	84	57	84	114	118 original
5202	44 [910; 2-Ketogluconic acid 129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	48	0.287	0.664	6.774	0.656	58	83	40	101	8	5 original
12335	44 [910; 2-Ketogluconic acid 19	Alanine (BP) (3TMS)	50	0.277	0.489	10.696	0.524	59	82	59	82	40	73 duplicate
5211	44 [910; 2-Ketogluconic acid 138	[674; Ergosterol (1TMS)]	34	0.273	0.362	17.688	0.447	60	81	66	75	92	100 original
5200	44 [910; 2-Ketogluconic acid 127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.271	0.497	7.750	0.538	61	80	56	85	15	65 original
5187	44 [910; 2-Ketogluconic acid 114	Fructose-6-phosphate	41	0.271	0.623	8.820	0.625	62	79	45	96	25	24 original
5176	44 [910; 2-Ketogluconic acid 103	[648; Ethylamine (2TMS)]	50	0.256	0.418	12.252	0.476	63	78	62	79	53	85 original
5156	44 [910; 2-Ketogluconic acid 83	Sorbitol	44	0.254	0.098	17.150	0.344	64	77	82	59	87	132 original
5165	44 [910; 2-Ketogluconic acid 92	[680; Glycerol-2-phosphate (4TMS)]	48	0.241	0.381	7.916	0.559	65	76	63	78	17	54 original
10671	44 [910; 2-Ketogluconic acid 6	Glycerol	50	0.221	0.429	35.491	0.622	66	75	61	80	140	26 duplicate
5144	44 [910; 2-Ketogluconic acid 71	[731; Erythrose (3TMS)]	50	0.216	0.341	10.454	0.498	67	74	68	73	39	78 original
5197	44 [910; 2-Ketogluconic acid 124	[734; 1-Monocetyl-glycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	45	0.204	0.139	24.297	0.414	68	73	79	62	123	116 original
5127	44 [910; 2-Ketogluconic acid 54	[NA]	49	0.199	0.544	10.962	0.585	69	72	54	87	42	39 original
14766	44 [910; 2-Ketogluconic acid 41	[639; Proline (2TMS)]	50	0.184	0.281	12.299	0.478	70	71	71	70	54	84 duplicate
5206	44 [910; 2-Ketogluconic acid 133	[855; Squalene]	50	0.182	0.209	10.250	0.379	71	70	76	65	35	124 original
5196	44 [910; 2-Ketogluconic acid 123	[945; Galactofuranose-6-phosphate (7TMS)]	50	0.158	0.369	10.314	0.553	72	68	65	76	36	57 original

5180	44 [910; 2-Ketogluconic acid 107	9-(Z)-Octadecenoic acid	50	0.158	0.103	11,840	0.406	73	69	81	60	49	119 original
5169	44 [910; 2-Ketogluconic acid 96	myo-Inositol	35	0.143	0.189	19,790	0.238	74	67	77	64	105	139 original
5174	44 [910; 2-Ketogluconic acid 101	Dopamine (4TMS)	50	0.141	0.216	11,528	0.420	75	66	74	67	45	113 original
5163	44 [910; 2-Ketogluconic acid 90	9-(Z)-Hexadecenoic acid (1TMS)	50	0.136	0.210	9,845	0.424	76	65	75	66	29	111 original
5170	44 [910; 2-Ketogluconic acid 97	756; beta-D-Methylglucopyranoside (4TMS)	48	0.115	0.150	18,236	0.560	77	64	78	63	95	51 original
5160	44 [910; 2-Ketogluconic acid 87	945; beta-D-Glucopyranose (5TMS)	48	0.101	0.357	31,837	0.588	78	63	67	74	136	36 original
5166	44 [910; 2-Ketogluconic acid 83	607; Putrescine (4TMS)	48	0.094	0.111	18,437	0.343	79	62	80	61	96	133 original
5189	44 [910; 2-Ketogluconic acid 116	682; Pseudouridine (5TMS)	21	0.076	0.687	9,716	0.515	80	61	37	104	30	76 original
5140	44 [910; 2-Ketogluconic acid 67	Citic acid	50	0.051	0.016	18,647	0.384	81	60	88	53	97	123 original
5125	44 [910; 2-Ketogluconic acid 52	[NA]	32	0.040	-0.284	21,764	0.598	82	59	108	35	112	31 original
5157	44 [910; 2-Ketogluconic acid 84	Mannitol	48	0.027	0.027	27,316	0.493	83	58	87	54	131	80 original
5164	44 [910; 2-Ketogluconic acid 91	766; beta-D-Methylglucopyranoside (4TMS)	50	0.025	0.092	17,409	0.427	84	57	83	58	89	108 original
5133	44 [910; 2-Ketogluconic acid 60	Glycerol-3-phosphate	50	-0.014	0.059	16,391	0.505	85	56	88	55	83	77 original
5152	44 [910; 2-Ketogluconic acid 79	Glucose	50	-0.019	0.234	30,687	0.593	86	55	73	68	135	32 original
14256	44 [910; 2-Ketogluconic acid 36	596; N-Acetylglutamic acid (2TMS)	50	-0.024	-0.079	22,921	0.450	87	54	92	49	115	98 duplicate
5209	44 [910; 2-Ketogluconic acid 136	748; D-Sedoheptulose-7-phosphate (7TMS)	17	-0.028	0.074	6,780	0.413	88	53	84	57	9	117 original
5212	44 [910; 2-Ketogluconic acid 139	700; Ergosta-5,7-dien-3-ol	27	-0.048	-0.068	19,858	0.385	89	52	90	51	106	122 original
5153	44 [910; 2-Ketogluconic acid 80	772; D-Glucose (5TMS)	48	-0.055	0.066	28,237	0.547	90	51	85	56	133	59 original
5203	44 [910; 2-Ketogluconic acid 130	Trehalose	49	-0.071	-0.075	23,467	0.451	91	50	91	50	121	97 original
5181	44 [910; 2-Ketogluconic acid 108	Octadecenoic acid	50	-0.115	-0.223	12,650	0.429	92	49	101	40	59	106 original
10805	44 [910; 2-Ketogluconic acid 7	Threonine	50	-0.117	-0.128	24,140	0.337	93	48	93	48	122	134 duplicate
5172	44 [910; 2-Ketogluconic acid 99	662; Ribose-5-phosphate methoxymine (BP) (5TMS)	36	-0.121	0.381	11,765	0.591	94	47	64	77	46	34 original
5126	44 [910; 2-Ketogluconic acid 53	Glycerol-2-phosphate	50	-0.138	-0.240	14,505	0.316	95	46	104	37	66	137 original
5131	44 [910; 2-Ketogluconic acid	636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)	50	-0.146	-0.152	15,129	0.399	96	45	94	47	70	120 original
10263	44 [910; 2-Ketogluconic acid 3	Ethanolamine	48	-0.147	-0.301	15,878	0.553	97	44	107	34	78	56 duplicate
14360	44 [910; 2-Ketogluconic acid 37	Phenylalanine	50	-0.159	-0.226	18,032	0.426	98	43	102	39	94	109 duplicate
5137	44 [910; 2-Ketogluconic acid 64	789; Tyramine (3TMS)	49	-0.167	-0.032	10,011	0.469	99	42	89	52	32	90 original
5148	44 [910; 2-Ketogluconic acid 75	Lysine	50	-0.174	-0.157	32,343	0.448	100	41	85	46	137	99 original
5191	44 [910; 2-Ketogluconic acid 118	928; Glucopyranose-6-phosphate (6TMS)	48	-0.180	-0.333	12,577	0.469	101	40	108	33	57	91 original
5139	44 [910; 2-Ketogluconic acid 66	Glyceric acid-3-phosphate	50	-0.195	-0.252	12,073	0.522	102	39	105	36	52	75 original
5136	44 [910; 2-Ketogluconic acid 63	Glutamine	38	-0.215	-0.376	19,437	0.587	103	38	112	29	101	37 original
5120	44 [910; 2-Ketogluconic acid 47	[NA]	50	-0.224	-0.430	15,158	0.571	104	37	114	27	71	47 original
10400	44 [910; 2-Ketogluconic acid 4	Phosphoric acid	38	-0.249	-0.206	27,051	0.357	105	36	99	42	130	127 duplicate
11070	44 [910; 2-Ketogluconic acid 9	Proline	49	-0.250	-0.219	23,439	0.356	106	35	100	41	120	129 duplicate
5168	44 [910; 2-Ketogluconic acid 95	770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)	36	-0.260	-0.509	19,095	0.437	107	34	120	21	99	103 original
5134	44 [910; 2-Ketogluconic acid 61	[NA]	50	-0.275	-0.197	10,845	0.454	108	33	98	43	41	94 original
11841	44 [910; 2-Ketogluconic acid 15	Alanine	50	-0.277	-0.188	17,457	0.591	109	32	86	45	91	35 duplicate
5154	44 [910; 2-Ketogluconic acid 81	Tyrosine	50	-0.278	-0.375	25,099	0.645	110	31	111	30	126	11 original
10125	44 [910; 2-Ketogluconic acid 2	Serine	48	-0.282	-0.229	18,778	0.355	111	30	103	38	98	130 duplicate
13721	44 [910; 2-Ketogluconic acid 31	622; Parabanic acid (2TMS)	50	-0.285	-0.427	15,759	0.476	112	29	113	28	77	86 duplicate
5132	44 [910; 2-Ketogluconic acid 59	Omitine; Arginine	50	-0.287	-0.353	32,912	0.422	113	28	109	32	138	112 original
5150	44 [910; 2-Ketogluconic acid	benzeneacetic acid methyl ester	48	-0.289	-0.373	23,004	0.372	114	27	110	31	116	125 original
10838	44 [910; 2-Ketogluconic acid 8	Isoleucine	41	-0.293	-0.191	17,844	0.298	115	26	97	44	83	138 duplicate
9986	44 [910; 2-Ketogluconic acid 1	938; Sulfuric acid (2TMS)	35	-0.314	-0.450	12,370	0.600	116	25	115	26	55	29 duplicate
5141	44 [910; 2-Ketogluconic acid 68	570; Hypoxanthine (2TMS)	9	-0.333	-0.765	14,517	0.113	117	24	137	4	67	140 original
5145	44 [910; 2-Ketogluconic acid 72	919; D-Xylopyranose (4TMS)	49	-0.338	-0.499	14,562	0.434	118	23	119	22	68	104 original
5121	44 [910; 2-Ketogluconic acid 48	Asparagine	50	-0.355	-0.675	15,604	0.578	119	22	128	13	74	45 original
11201	44 [910; 2-Ketogluconic acid 10	Glycine	50	-0.357	-0.721	15,978	0.667	120	21	133	8	81	2 duplicate
13830	44 [910; 2-Ketogluconic acid 32	728; N,N-Dimethyllysine methyl ester]	49	-0.381	-0.548	22,028	0.475	121	19	121	20	113	87 duplicate

5162	44 [910; 2-Ketogluconic acid]	89 [775; Dopamine (4TMS)]	21 -0.381	-0.681	19,249	0.431	122	20	128	12	100	105 original
13275	44 [910; 2-Ketogluconic acid]	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	39 -0.382	-0.654	23,300	0.454	123	18	126	15	119	95-juplicate
14045	44 [910; 2-Ketogluconic acid]	34 Aspartic acid	50 -0.385	-0.469	26,683	0.350	124	17	118	25	128	131-juplicate
13611	44 [910; 2-Ketogluconic acid]	30 [815; Ethyl-3(2H)-thiophenone]	50 -0.412	-0.487	24,740	0.327	125	16	117	24	124	136-juplicate
5124	44 [910; 2-Ketogluconic acid]	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	30 -0.416	-0.611	19,625	0.395	126	15	124	17	104	121 original
12813	44 [910; 2-Ketogluconic acid]	23 Homoserine	50 -0.420	-0.682	16,407	0.469	127	14	130	11	84	89-juplicate
13938	44 [910; 2-Ketogluconic acid]	33 Methionine	50 -0.443	-0.571	16,179	0.356	128	13	122	19	82	128-juplicate
14865	44 [910; 2-Ketogluconic acid]	42 Glutamic acid	46 -0.447	-0.485	25,001	0.333	129	12	118	23	125	135-juplicate
5128	44 [910; 2-Ketogluconic acid]	55 [612; 4-Aminobutyric acid (2TBS)]	29 -0.473	-0.638	23,238	0.486	130	11	125	16	118	82 original
5142	44 [910; 2-Ketogluconic acid]	69 Arginine	46 -0.474	-0.705	19,465	0.495	131	10	131	10	102	79 original
5118	44 [910; 2-Ketogluconic acid]	45 Homocysteine	47 -0.512	-0.666	23,234	0.418	132	9	127	14	117	114 original
5204	44 [910; 2-Ketogluconic acid]	131 [626; 5-Methylthioadenosine (3TMS)]	43 -0.515	-0.717	19,594	0.564	133	8	132	9	103	49 original
14963	44 [910; 2-Ketogluconic acid]	43 [548; Leucine (2TBS)]	46 -0.515	-0.591	12,752	0.367	134	7	123	18	60	126-juplicate
5171	44 [910; 2-Ketogluconic acid]	98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	35 -0.523	-0.755	20,589	0.464	135	6	135	6	108	92 original
10538	44 [910; 2-Ketogluconic acid]	5 Leucine	31 -0.527	-0.796	16,857	0.427	136	5	138	3	86	107-juplicate
13046	44 [910; 2-Ketogluconic acid]	25 [709; 2,5-Diaminovelarolactam (2TMS)]	45 -0.541	-0.743	21,079	0.598	137	4	134	7	110	30-juplicate
5122	44 [910; 2-Ketogluconic acid]	49 [877; Pyrophosphoric acid (4TMS)]	50 -0.603	-0.758	25,594	0.523	138	3	136	5	127	74 original
12456	44 [910; 2-Ketogluconic acid]	20 [619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	17 -0.618	-0.841	15,628	0.470	139	2	139	2	75	88-juplicate
5155	44 [910; 2-Ketogluconic acid]	82 Lysine	25 -0.693	-0.812	15,766	0.578	140	1	140	1	76	44 original
13939	45 Homocysteine	33 Methionine	61 0.662	0.708	22,560	0.483	1	140	4	137	65	12-juplicate
13912	45 Homocysteine	30 [815; Ethyl-3(2H)-thiophenone]	61 0.663	0.650	45,782	0.482	2	139	9	132	124	13-juplicate
5237	45 Homocysteine	68 [570; Hypoxanthine (2TMS)]	19 0.637	0.714	4,088	0.476	3	138	3	138	1	17 original
5251	45 Homocysteine	82 Lysine	37 0.613	0.793	26,701	0.497	4	137	1	140	81	10 original
10537	45 Homocysteine	5 Leucine	43 0.608	0.744	13,613	0.543	5	136	2	139	28	1-juplicate
5258	45 Homocysteine	89 [775; Dopamine (4TMS)]	34 0.608	0.634	13,712	0.427	6	135	13	128	29	63 original
14046	45 Homocysteine	84 Aspartic acid	61 0.574	0.682	49,243	0.521	7	134	6	135	132	4-juplicate
13047	45 Homocysteine	25 [709; 2,5-Diaminovelarolactam (2TMS)]	45 0.574	0.672	15,795	0.460	8	133	8	133	34	25-juplicate
5238	45 Homocysteine	69 Arginine	57 0.559	0.679	35,513	0.513	9	132	7	134	109	6 original
5220	45 Homocysteine	71 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	43 0.557	0.650	5,834	0.538	10	131	10	131	5	3 original
5246	45 Homocysteine	77 [826; beta-[(5-methyl-2-thienyl)methyl]amino-benzeneacetic acid methyl ester]	59 0.531	0.576	44,589	0.478	11	130	18	123	122	16 original
11202	45 Homocysteine	10 Glycine	61 0.528	0.639	34,600	0.463	12	129	12	129	105	20-juplicate
5217	45 Homocysteine	48 Asparagine	61 0.525	0.686	22,308	0.459	13	128	5	136	64	27 original
10939	45 Homocysteine	8 Isoleucine	52 -0.523	0.196	31,478	0.412	14	127	42	99	85	85-juplicate
11071	45 Homocysteine	9 Proline	60 0.512	0.388	41,994	0.417	15	126	33	108	119	74-juplicate
5228	45 Homocysteine	59 Ornithine; Arginine	61 0.507	0.548	57,303	0.429	16	125	22	119	138	60 original
14866	45 Homocysteine	42 Glutamic acid	57 0.503	0.550	43,615	0.493	17	124	21	120	121	11-juplicate
12814	45 Homocysteine	23 Homoserine	61 0.494	0.650	22,766	0.463	18	123	11	130	68	21-juplicate
5218	45 Homocysteine	49 [877; Pyrophosphoric acid (4TMS)]	61 0.486	0.630	10,493	0.406	19	121	14	127	16	90 original
5250	45 Homocysteine	81 Tyrosine	61 0.486	0.497	49,908	0.460	20	122	25	118	133	24 original
13831	45 Homocysteine	32 [729; N,N-Dimethyllysine methyl ester]	60 0.476	0.574	16,590	0.509	21	120	19	122	38	7-juplicate
5264	45 Homocysteine	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	49 0.461	0.592	5,767	0.413	22	119	16	125	4	73 original
5230	45 Homocysteine	61 [NA]	61 0.457	0.509	20,141	0.384	23	118	24	117	56	99 original
14361	45 Homocysteine	37 Phenylalanine	61 0.454	0.487	39,322	0.413	24	117	26	115	115	83-juplicate
13722	45 Homocysteine	31 [622; Parabenic acid (2TMS)]	61 0.445	0.480	13,440	0.480	25	116	28	113	26	15-juplicate
5224	45 Homocysteine	55 [612; 4-Aminobutyric acid (2TBS)]	41 0.437	0.469	8,451	0.437	26	115	30	111	13	49 original
10264	45 Homocysteine	3 Ethanolamine	59 0.431	0.478	13,412	0.407	27	114	29	112	25	88-juplicate
10126	45 Homocysteine	2 Serine	59 0.402	0.299	32,235	0.445	28	113	37	104	98	40-juplicate
13276	45 Homocysteine	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	52 0.398	0.606	13,150	0.540	29	112	15	126	23	2-juplicate
14964	45 Homocysteine	43 [548; Leucine (2TBS)]	58 0.393	0.591	21,385	0.450	30	111	17	124	61	34-juplicate

5267	45 Homocysteine	98	[697; Ribose-5-phosphate methoxamine (5TMS)]	47	0.391	0.529	6.955	0.481	31	110	23	118	9	14 original
5300	45 Homocysteine	131	[626; 5-Methylthiadenosine (3TMS)]	53	0.364	0.485	6.683	0.413	32	109	27	114	7	82 original
5232	45 Homocysteine	63	Glutamine	49	0.357	0.456	18.401	0.387	33	108	31	110	49	97 original
10806	45 Homocysteine	7	Theonine	61	0.345	0.343	46.814	0.428	34	108	35	108	127	84 duplicate
5235	45 Homocysteine	66	Glycic acid-3-phosphate	61	0.345	0.321	17.257	0.459	35	107	36	105	41	28 original
5236	45 Homocysteine	67	Citic acid	61	0.313	0.348	40.447	0.381	36	105	34	107	116	103 original
5221	45 Homocysteine	52	[NA]	43	0.309	0.432	10.876	0.438	37	104	32	109	17	54 original
12457	45 Homocysteine	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	0.295	0.551	7.823	0.504	38	103	20	121	12	9 duplicate
5229	45 Homocysteine	60	Glycerol-3-phosphate	61	0.258	0.265	37.929	0.367	39	102	39	102	114	111 original
5244	45 Homocysteine	75	Lysine	61	0.173	0.247	56.022	0.417	40	101	40	101	137	75 original
5240	45 Homocysteine	71	[731; Erythrose (3TMS)]	61	0.121	0.037	28.342	0.421	41	100	49	92	88	71 original
5227	45 Homocysteine	58	[636; 4R-Acetalido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	61	0.117	0.214	31.782	0.377	42	99	41	100	96	105 original
5262	45 Homocysteine	93	[607; Putrescine (4TMS)]	57	0.115	0.116	11.084	0.305	43	98	44	97	18	135 original
14257	45 Homocysteine	36	[596; N-Acetylglutamic acid (2TMS)]	61	0.114	0.043	44.878	0.404	44	97	47	94	123	82 duplicate
5305	45 Homocysteine	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	15	0.105	0.279	12.078	0.373	45	96	38	103	19	108 original
5277	45 Homocysteine	108	Octadecenoic acid	61	0.090	0.092	17.607	0.331	46	95	46	95	43	130 original
10401	45 Homocysteine	4	Phosphoric acid	48	0.057	0.126	47.274	0.334	47	94	43	98	128	129 duplicate
5241	45 Homocysteine	72	[919; D-Xylopyranose (4TMS)]	60	0.036	0.094	17.891	0.343	48	93	45	96	46	122 original
9987	45 Homocysteine	1	[938; Sulfuric acid (2TMS)]	33	0.034	0.032	17.233	0.416	49	92	50	91	40	79 duplicate
5299	45 Homocysteine	130	Trehalose	60	0.000	-0.048	46.502	0.368	50	91	56	85	126	110 original
5253	45 Homocysteine	84	Mannitol	60	-0.008	-0.057	48.043	0.410	51	90	57	84	129	87 original
5233	45 Homocysteine	64	[789; Tyramine (3TMS)]	60	-0.021	-0.014	19.672	0.336	52	89	54	87	50	127 original
5208	45 Homocysteine	119	[931; myo-Inositol-2-phosphate (7TMS)]	61	-0.026	-0.057	22.647	0.368	53	88	58	83	67	109 original
5388	45 Homocysteine	139	[700; Ergosta-5,7-dien-3-ol]	35	-0.032	-0.007	5.149	0.235	54	87	53	88	2	140 original
5276	45 Homocysteine	107	8-(Z)-Octadecenoic acid	61	-0.039	0.012	31.073	0.314	55	86	52	89	94	133 original
5293	45 Homocysteine	124	[734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]	56	-0.045	-0.083	6.954	0.339	56	85	59	82	8	128 original
5216	45 Homocysteine	47	[NA]	61	-0.056	0.022	22.891	0.387	57	83	51	90	69	98 original
11842	45 Homocysteine	15	Alanine	61	-0.056	-0.133	34.939	0.422	58	84	62	79	107	69 duplicate
5296	45 Homocysteine	127	[777; Fructose-6-phosphate methoxamine (6TMS)]	36	-0.067	-0.178	17.762	0.342	59	82	67	74	45	124 original
5222	45 Homocysteine	53	Glycerol-2-phosphate	61	-0.071	-0.034	12.822	0.312	60	80	55	88	21	134 original
5259	45 Homocysteine	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	61	-0.071	-0.086	22.565	0.359	61	81	60	81	68	113 original
5280	45 Homocysteine	111	[583; Erythritol (4TMS)]	39	-0.093	-0.129	5.458	0.288	62	79	61	80	3	137 original
5252	45 Homocysteine	83	Sorbitol	55	-0.099	0.040	35.649	0.353	63	78	48	93	110	116 original
5287	45 Homocysteine	118	[928; Glucopyranose-6-phosphate (6TMS)]	55	-0.104	-0.170	18.021	0.317	64	77	68	75	47	132 original
5297	45 Homocysteine	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	42	-0.127	-0.181	22.083	0.348	65	76	68	73	63	121 original
5306	45 Homocysteine	137	Ergosterol	61	-0.142	-0.162	29.528	0.353	66	75	64	77	91	115 original
5260	45 Homocysteine	91	[766; beta-D-Methylglucopyranoside (4TMS)]	61	-0.158	-0.139	28.903	0.375	67	74	63	78	90	108 original
5266	45 Homocysteine	49	[756; beta-D-Methylglucopyranoside (4TMS)]	49	-0.168	-0.240	35.321	0.382	68	73	71	70	108	101 original
5274	45 Homocysteine	105	[705; 2-Ketogluconic acid (5TMS)]	45	-0.172	-0.231	25.144	0.349	69	72	70	71	79	119 original
5248	45 Homocysteine	79	Glucose	61	-0.184	-0.374	51.600	0.396	70	71	82	59	138	94 original
5307	45 Homocysteine	138	[674; Ergosterol (1TMS)]	43	-0.192	-0.321	8.493	0.287	71	70	75	66	14	138 original
5310	45 Homocysteine	141	Lanosta-8,24-dien-3-beta-ol	58	-0.204	-0.328	12.093	0.343	72	69	76	65	20	123 original
5302	45 Homocysteine	133	[855; Squalene]	61	-0.208	-0.253	21.957	0.341	73	68	72	69	62	125 original
5304	45 Homocysteine	135		61	-0.223	-0.338	28.629	0.378	74	67	78	63	89	104 original
5270	45 Homocysteine	101	[832; Dopamine (4TMS)]	61	-0.224	-0.201	24.326	0.374	75	66	69	72	76	107 original
5283	45 Homocysteine	94	Hexadecanoic acid	61	-0.231	-0.495	37.923	0.413	76	65	90	51	113	84 original
5309	45 Homocysteine	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	48	-0.231	-0.295	7.676	0.298	77	64	74	67	10	136 original



5265	45 Homocysteine	96	myo-Inositol	46	-0.235	-0.168	5.957	0.336	78	63	65	76	6	128 original
5261	45 Homocysteine	92	[880; Ribitol-2-phosphate (4TMS)]	51	-0.236	-0.347	20.696	0.323	79	62	79	62	57	131 original
5268	45 Homocysteine	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	38	-0.249	-0.498	15.029	0.413	80	61	91	50	31	81 original
5285	45 Homocysteine	116	[882; Pseudouridine (5TMS)]	27	-0.264	-0.288	13.973	0.252	81	60	73	68	30	139 original
5278	45 Homocysteine	109	Octadecanoic acid	61	-0.259	-0.561	37.802	0.425	82	59	103	38	112	65 original
5249	45 Homocysteine	80	[772; D-Glucose (5TMS)]	59	-0.268	-0.477	46.488	0.387	83	58	89	52	125	95 original
5223	45 Homocysteine	54	[NA]	52	-0.268	-0.386	16.528	0.350	84	57	83	58	37	118 original
5254	45 Homocysteine	85	[523; Methylcitric acid (4TMS)]	45	-0.271	-0.538	16.650	0.450	85	56	97	44	39	33 original
5272	45 Homocysteine	103	[648; Ethylamine (2TMS)]	60	-0.278	-0.333	27.699	0.428	86	55	77	64	85	61 original
5271	45 Homocysteine	102	[904; Galactose methoxyamine (5TMS)]	61	-0.284	-0.361	17.623	0.398	87	54	81	60	44	93 original
5292	45 Homocysteine	123	[945; Galactofuranose-6-phosphate (7TMS)]	61	-0.289	-0.427	27.043	0.428	88	53	85	58	82	62 original
5281	45 Homocysteine	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	60	-0.308	-0.440	7.758	0.410	89	52	86	55	11	88 original
5269	45 Homocysteine	100	[857; Mannitol (6TMS)]	61	-0.311	-0.454	24.798	0.421	90	51	87	54	77	70 original
5282	45 Homocysteine	113	Galactose-6-phosphate	59	-0.326	-0.510	18.337	0.382	91	50	93	48	48	102 original
5283	45 Homocysteine	114	Fructose-6-phosphate	50	-0.326	-0.511	15.982	0.348	92	49	94	47	35	120 original
11461	45 Homocysteine	12	Glycercic acid	60	-0.350	-0.538	13.453	0.416	93	48	98	43	27	77 duplicate
5266	45 Homocysteine	57	[757; 2-Deoxy-pentose-3-yose dimethoxyamine (2TMS)]	52	-0.354	-0.561	27.551	0.407	94	47	104	37	84	89 original
5225	45 Homocysteine	56	[829; Orotic acid (3TMS)]	61	-0.357	-0.571	21.050	0.429	95	46	107	34	58	59 original
13501	45 Homocysteine	29	Erythritol	61	-0.360	-0.552	19.636	0.474	96	45	101	40	53	18 duplicate
12091	45 Homocysteine	17	[700; 2-methyl-1,2-propanediol (2TMS)]	61	-0.363	-0.520	34.295	0.424	97	44	96	45	104	67 duplicate
14767	45 Homocysteine	41	[639; Proline (2TMS)]	61	-0.373	-0.468	30.033	0.416	98	43	88	53	92	78 duplicate
11967	45 Homocysteine	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	61	-0.381	-0.585	34.609	0.440	99	42	112	29	106	46 duplicate
5258	45 Homocysteine	87	[945; beta-D-Glucopyranose (5TMS)]	59	-0.382	-0.505	51.435	0.353	100	41	92	49	135	117 original
12931	45 Homocysteine	24	[725; 2-Ketocetonic acid (2TMS)]	61	-0.390	-0.611	48.919	0.433	101	40	115	26	131	57 duplicate
5273	45 Homocysteine	104	[795; Erythritol (4TMS)]	60	-0.391	-0.639	21.252	0.439	102	39	127	14	60	47 original
11332	45 Homocysteine	11	Succinic acid	61	-0.391	-0.541	23.637	0.436	103	38	100	41	74	53 duplicate
5303	45 Homocysteine	134	Isomaltose	61	-0.396	-0.611	41.494	0.440	104	37	116	25	118	43 original
10672	45 Homocysteine	6	Glycerol	61	-0.398	-0.518	58.438	0.416	105	36	95	46	140	76 duplicate
5239	45 Homocysteine	70	[893; 2-Furan-2-hydroxyacetic acid (2TMS)]	54	-0.399	-0.408	33.587	0.358	106	35	84	57	103	114 original
5289	45 Homocysteine	120	[945; Uridine (3TMS)]	51	-0.405	-0.351	27.130	0.451	107	34	80	61	83	32 original
5243	45 Homocysteine	74	[912; Tetradecanoic acid (1TMS)]	61	-0.412	-0.628	21.181	0.461	108	33	123	18	59	23 original
14484	45 Homocysteine	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	61	-0.413	-0.622	23.481	0.437	109	32	121	20	73	51 duplicate
5257	45 Homocysteine	88	Gluconic acid	61	-0.414	-0.574	27.828	0.440	110	30	109	32	86	44 original
12214	45 Homocysteine	18	[590; 1-Acetyl-2-thiohydantoin]	61	-0.414	-0.620	23.479	0.430	111	31	120	21	72	58 duplicate
5215	45 Homocysteine	39	Arabinose	61	-0.417	-0.594	32.574	0.434	112	29	113	28	99	55 original
14566	45 Homocysteine	13	Uracil	60	-0.423	-0.630	31.806	0.444	113	28	124	17	97	41 duplicate
11589	45 Homocysteine	65	[829; 1-Phenylethanol (1TMS)]	61	-0.424	-0.617	32.871	0.437	114	27	118	23	100	50 duplicate
5234	45 Homocysteine	132	[846; 3-Deoxyglucitol (5TMS)]	60	-0.425	-0.620	23.451	0.447	115	26	119	22	71	36 original
5301	45 Homocysteine	35	[895; Isomaltose methoxyamine (8TMS)]	39	-0.428	-0.565	16.130	0.406	116	25	105	36	36	91 original
14152	45 Homocysteine	33	Pyroglutamic acid	61	-0.442	-0.554	57.974	0.385	117	24	102	39	139	98 duplicate
13162	45 Homocysteine	26	Citramalic acid	61	-0.444	-0.599	33.016	0.424	118	23	114	27	101	66 duplicate
5242	45 Homocysteine	73	[708; Glucose methoxyamine (5TMS)]	54	-0.444	-0.632	18.990	0.449	119	22	125	16	51	35 original
5298	45 Homocysteine	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	56	-0.447	-0.633	23.885	0.434	120	21	128	15	75	56 original
12338	45 Homocysteine	19	Alanine (BP) (3TMS)	61	-0.447	-0.573	28.083	0.422	121	20	108	33	87	68 duplicate
5231	45 Homocysteine	62	[812; D-Xylofuranose (4TMS)]	61	-0.450	-0.575	30.797	0.437	122	19	110	31	93	52 original
5284	45 Homocysteine	115	Glucose-6-phosphate	59	-0.452	-0.566	41.204	0.383	123	18	108	35	117	100 original
13389	45 Homocysteine	28	Malic acid	61	-0.457	-0.644	25.521	0.459	124	17	130	11	80	26 duplicate
12696	45 Homocysteine	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	51	-0.457	-0.579	13.138	0.451	125	16	111	30	22	31 duplicate
11716	45 Homocysteine	14	Fumaric acid	61	-0.477	-0.640	15.200	0.458	126	15	128	13	32	29 duplicate

5295	45 Homocysteine	126 [559; Erythritol (4TMS)]	42 -0.477	-0.615	17.274	0.438	127	14	117	24	42	48 original
5255	45 Homocysteine	86 [793; D-Galactono-1,4-lactone (4TMS)]	58 -0.483	-0.627	35.992	0.461	128	13	122	19	111	22 original
5294	45 Homocysteine	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	61 -0.491	-0.541	48.638	0.384	129	12	99	42	130	112 original
12577	45 Homocysteine	21 [878; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	61 -0.502	-0.694	33.320	0.447	130	11	136	5	102	37 duplicate
15061	45 Homocysteine	44 [910; 2-Ketogluconic acid methoxymine (4TMS)]	47 -0.512	-0.666	23.234	0.418	131	10	132	9	70	72 duplicate
5219	45 Homocysteine	50 [746; Ribonic acid-1,4-lactone (3TMS)]	58 -0.515	-0.646	9.959	0.440	132	9	131	10	15	45 original
5247	45 Homocysteine	78 Mannose	59 -0.528	-0.687	19.743	0.443	133	8	133	8	54	42 original
5291	45 Homocysteine	122 [844; Erythritol (4TMS)]	49 -0.529	-0.689	15.600	0.447	134	7	134	7	33	38 original
5279	45 Homocysteine	110 [715; Erythritol (4TMS)]	51 -0.537	-0.693	19.599	0.467	135	6	135	6	52	19 original
5286	45 Homocysteine	117 [724; Glycerol (3TMS)]	53 -0.546	-0.731	19.798	0.445	136	5	137	4	55	39 original
5290	45 Homocysteine	121 [657; Erythritol (4TMS)]	52 -0.549	-0.735	13.332	0.452	137	4	138	3	24	30 original
5245	45 Homocysteine	76 Fructose	61 -0.550	-0.841	42.052	0.413	138	3	129	12	120	80 original
14667	45 Homocysteine	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	61 -0.573	-0.776	51.190	0.519	139	2	140	1	134	5 duplicate
5275	45 Homocysteine	106 [733; Threitol (4TMS)]	59 -0.580	-0.742	25.125	0.504	140	1	139	2	78	8 original
5321	46 Arabinose	757; 2-Desoxy-pentose-3-ylose dimethoxymine (2TMS)]	55 0.887	0.991	7.306	0.714	1	140	2	139	3	7 original
12932	46 Arabinose	24 [725; 2-Ketocacetic acid (2TMS)]	64 0.874	0.980	22.367	0.725	2	139	6	135	86	3 duplicate
5329	46 Arabinose	65 [846; 3-Deoxyglucitol (5TMS)]	63 0.873	0.989	11.854	0.738	3	138	5	136	17	1 original
5393	46 Arabinose	129 [840; Maltose methoxymine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59 0.868	0.979	10.486	0.688	4	137	7	134	10	13 original
11968	46 Arabinose	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	64 0.862	0.963	11.148	0.705	5	136	9	132	14	9 duplicate
5320	46 Arabinose	64 [829; Orotic acid (3TMS)]	64 0.859	0.992	12.722	0.723	6	135	1	140	24	5 original
5350	46 Arabinose	86 [793; D-Galactono-1,4-lactone (4TMS)]	61 0.858	0.991	5.924	0.719	7	134	3	138	2	6 original
5398	46 Arabinose	134 Isomaltose	64 0.850	0.990	11.265	0.734	8	133	4	137	15	2 original
11590	46 Arabinose	13 Urcil	64 0.840	0.988	7.877	0.695	9	132	8	133	4	11 duplicate
5314	46 Arabinose	50 [746; Ribonic acid-1,4-lactone (3TMS)]	61 0.808	0.931	27.190	0.624	10	131	16	125	115	45 original
12092	46 Arabinose	17 [700; 2-methyl-1,2-propanediol (2TMS)]	64 0.794	0.938	10.024	0.617	11	130	13	128	9	52 duplicate
14667	46 Arabinose	39 [829; 1-Phenylethanol (1TMS)]	63 0.790	0.951	4.896	0.677	12	129	11	130	1	20 duplicate
13502	46 Arabinose	28 Erythritol	64 0.780	0.924	15.591	0.662	13	128	17	124	45	24 duplicate
5352	46 Arabinose	89 Gluconic acid	64 0.778	0.922	7.930	0.680	14	127	18	123	5	17 original
5318	46 Arabinose	54 [NA]	55 0.770	0.952	18.578	0.626	15	126	10	131	61	43 original
5363	46 Arabinose	99 [662; Ribose-5-phosphate methoxymine (BP) (5TMS)]	41 0.751	0.907	18.004	0.679	16	125	20	121	66	19 original
14465	46 Arabinose	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	64 0.738	0.939	12.266	0.661	17	124	12	129	21	26 duplicate
5326	46 Arabinose	62 [812; D-Xylofuranose (4TMS)]	64 0.728	0.936	12.244	0.669	18	123	14	127	20	22 original
11333	46 Arabinose	11 Succinic acid	64 0.707	0.904	13.063	0.627	19	122	21	120	27	42 duplicate
5367	46 Arabinose	103 [648; Ethylamine (2TMS)]	63 0.668	0.835	8.439	0.568	20	121	34	107	7	64 original
5356	46 Arabinose	92 [680; Glyceral-2-phosphate (4TMS)]	54 0.667	0.882	13.479	0.613	21	120	25	116	29	54 original
12697	46 Arabinose	22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52 0.633	0.877	19.322	0.621	22	119	29	112	70	48 duplicate
11717	46 Arabinose	14 Fumaric acid	64 0.628	0.900	18.923	0.645	23	118	23	118	64	34 duplicate
5369	46 Arabinose	105 [705; 2-Ketogluconic acid (5TMS)]	48 0.622	0.879	10.867	0.623	24	117	28	113	12	46 original
5337	46 Arabinose	73 [708; Glucose methoxymine (5TMS)]	57 0.622	0.805	12.816	0.541	25	116	40	101	26	74 original
5361	46 Arabinose	97 [756; beta-D-Methylglucopyranoside (4TMS)]	52 0.614	0.843	8.703	0.571	26	115	33	108	6	63 original
5340	46 Arabinose	76 Fructose	64 0.610	0.835	14.262	0.569	27	114	15	126	36	23 original
11462	46 Arabinose	12 Glyceric acid	63 0.607	0.823	20.717	0.595	28	113	38	103	75	58 duplicate
5342	46 Arabinose	78 Mannose	62 0.585	0.851	14.911	0.587	29	112	32	109	39	61 original
13390	46 Arabinose	28 Malic acid	64 0.582	0.895	12.770	0.649	30	111	24	117	25	32 duplicate
14668	46 Arabinose	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	64 0.578	0.831	27.881	0.633	31	110	35	106	118	38 duplicate
5389	46 Arabinose	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64 0.577	0.881	21.327	0.631	32	109	27	114	79	41 original
9988	46 Arabinose	1 [938; Sulfuric acid (2TMS)]	36 0.575	0.892	16.915	0.649	33	108	53	88	50	33 duplicate
5334	46 Arabinose	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57 0.566	0.871	13.933	0.523	34	107	56	85	35	82 original
5365	46 Arabinose	101 [832; Dopamine (4TMS)]	64 0.557	0.743	12.059	0.533	35	106	48	93	19	78 original

5370	46 Arabinose	106 [733; Threitol (4TMS)]	62 0.551	0.875	9,729	0.703	38	105	31	110	8	10 original
5355	46 Arabinose	91 [766; beta-D-Methylglucopyranoside (4TMS)]	64 0.549	0.702	13,469	0.498	37	104	52	89	28	93 original
14153	46 Arabinose	35 Pyroglutamic acid	64 0.541	0.913	32,803	0.655	38	103	19	122	133	29 duplicate
12578	46 Arabinose	21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64 0.520	0.748	13,632	0.667	39	102	47	94	32	66 duplicate
5378	46 Arabinose	115 Glucose-6-phosphate	62 0.511	0.900	15,933	0.658	40	101	22	119	46	27 original
5392	46 Arabinose	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45 0.509	0.876	10,979	0.631	41	100	30	111	13	40 original
5384	46 Arabinose	120 [945; Uridine (3TMS)]	54 0.493	0.342	12,310	0.636	42	99	71	70	22	37 original
5351	46 Arabinose	87 [945; beta-D-Glucopyranose (5TMS)]	62 0.481	0.813	25,200	0.560	43	98	39	102	89	68 original
13163	46 Arabinose	26 Citramalic acid	64 0.469	0.757	15,043	0.525	44	97	43	98	41	81 duplicate
10673	46 Arabinose	6 Glycerol	64 0.442	0.785	33,810	0.568	45	96	42	99	136	65 duplicate
5366	46 Arabinose	102 [904; Galactose methoxamine (5TMS)]	64 0.427	0.635	17,609	0.529	46	95	59	82	58	80 original
5364	46 Arabinose	100 [857; Mannitol (6TMS)]	64 0.423	0.703	13,543	0.529	47	94	51	90	31	79 original
5376	46 Arabinose	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63 0.422	0.650	26,940	0.534	48	93	58	83	114	77 original
5381	46 Arabinose	117 [724; Glycerol (3TMS)]	56 0.412	0.755	15,001	0.592	49	92	45	96	40	59 original
5374	46 Arabinose	110 [715; Erythritol (4TMS)]	54 0.412	0.828	17,202	0.681	50	91	36	105	51	16 original
5366	46 Arabinose	122 [644; Erythritol (4TMS)]	52 0.410	0.828	23,387	0.609	51	90	37	104	89	55 original
5396	46 Arabinose	132 [895; Isomaltose methoxamine (6TMS)]	42 0.405	0.882	22,172	0.653	52	89	26	115	85	31 original
5385	46 Arabinose	121 [657; Erythritol (4TMS)]	55 0.405	0.728	22,936	0.605	53	88	49	92	88	56 original
5349	46 Arabinose	85 [529; Methylcitric acid (4TMS)]	48 0.395	0.626	11,378	0.450	54	87	60	81	16	114 original
15062	46 Arabinose	44 [910; 2-Ketogluconic acid methoxamine (4TMS)]	50 0.355	0.755	12,455	0.633	55	86	46	95	23	39 duplicate
5399	46 Arabinose	[902; Melibiose (6TMS); alpha-D-Gal-(1,6)-D-Glc (6TMS)]	64 0.334	0.505	14,686	0.490	56	85	66	75	38	98 original
5377	46 Arabinose	113 Galactose-6-phosphate	62 0.309	0.787	16,064	0.587	57	84	41	100	47	80 original
12215	46 Arabinose	18 [590; 1-Acetyl-2-thiohydantoin]	64 0.302	0.537	14,845	0.446	58	83	62	79	37	117 duplicate
5344	46 Arabinose	80 [772; D-Glucose (5TMS)]	62 0.290	0.707	21,650	0.508	59	82	50	91	84	90 original
5368	46 Arabinose	104 [795; Erythritol (4TMS)]	63 0.259	0.528	15,143	0.547	60	81	65	76	42	72 original
12337	46 Arabinose	19 Alanine (BP) (3TMS)	64 0.258	0.672	12,058	0.557	61	80	55	86	18	70 duplicate
5391	46 Arabinose	127 [777; Fructose-6-phosphate methoxamine (6TMS)]	39 0.258	0.677	15,153	0.684	62	79	54	87	43	14 original
5338	46 Arabinose	74 [912; Tetradecanoic acid (1TMS)]	64 0.255	0.536	16,684	0.473	63	78	63	78	49	107 original
5348	46 Arabinose	84 Mannitol	62 0.225	0.455	24,538	0.458	64	77	68	73	96	111 original
5380	46 Arabinose	116 [882; Pseudouridine (5TMS)]	30 0.209	0.267	13,484	0.483	65	76	74	67	30	103 original
5378	46 Arabinose	114 Fructose-6-phosphate	53 0.205	0.756	17,452	0.618	66	75	44	97	53	49 original
5390	46 Arabinose	126 [559; Erythritol (4TMS)]	45 0.202	0.551	18,053	0.656	67	74	61	80	60	28 original
5311	46 Arabinose	47 [NA]	64 0.188	0.239	17,974	0.458	68	73	77	64	58	112 original
14768	46 Arabinose	41 [639; Proline (2TMS)]	64 0.186	0.497	13,738	0.488	69	72	67	74	34	100 duplicate
5360	46 Arabinose	96 myo-Inositol	49 0.177	0.213	26,631	0.369	70	71	78	63	108	136 original
5387	46 Arabinose	93 [607; Putrescine (4TMS)]	60 0.167	0.252	26,056	0.429	71	70	75	68	105	128 original
5357	46 Arabinose	123 [945; Galactofuranose-6-phosphate (7TMS)]	64 0.163	0.529	13,734	0.560	72	69	64	77	33	69 original
5347	46 Arabinose	83 Sorbitol	58 0.132	-0.289	21,571	0.356	73	68	91	50	83	137 original
5343	46 Arabinose	79 Glucose	64 0.117	0.650	26,649	0.616	74	67	57	84	109	53 original
11843	46 Arabinose	15 Alanine	64 0.102	0.445	15,263	0.682	75	66	69	72	44	15 duplicate
5375	46 Arabinose	111 [583; Erythritol (4TMS)]	42 0.089	0.282	30,228	0.444	76	65	73	68	123	118 original
5328	46 Arabinose	64 [789; Tyramine (3TMS)]	63 0.086	0.352	17,542	0.436	77	64	70	71	54	122 original
5317	46 Arabinose	53 Glycerol-2-phosphate	64 0.044	-0.086	22,936	0.371	78	63	84	57	87	134 original
5397	46 Arabinose	133 [855; Squalene]	64 0.040	0.014	17,987	0.369	79	62	81	60	57	135 original
5354	46 Arabinose	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	64 0.016	-0.118	17,569	0.438	80	61	85	56	55	121 original
5404	46 Arabinose	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49 0.015	0.126	24,056	0.491	81	60	80	61	92	97 original
5373	46 Arabinose	109 Octadecanoic acid	64 -0.006	0.309	18,739	0.493	82	59	72	69	63	96 original
5327	46 Arabinose	63 Glutamine	58 -0.039	-0.770	30,452	0.723	83	58	123	18	126	4 original
5382	46 Arabinose	118 [928; Glucopyranose-6-phosphate (6TMS)]	58 -0.041	0.251	19,139	0.454	84	57	76	65	68	113 original
5405	46 Arabinose	141 Lanosta-8,24-dien-3-beta-ol	61 -0.055	-0.027	24,346	0.488	85	56	83	58	95	99 original

5358	46 Arabinose	94	Hexadecanoic acid	64	-0.068	0.199	18.712	0.483	86	55	79	62	82	104 original
5356	46 Arabinose	72	[919; D-Xylopyranose (4TMS)]	63	-0.097	-0.156	21.143	0.341	87	54	86	55	77	138 original
5383	46 Arabinose	119	[931; myo-Inositol-2-phosphate (7TMS)]	64	-0.123	-0.252	18.984	0.514	88	53	89	52	65	86 original
5403	46 Arabinose	139	[700; Ergosta-5,7-dien-3-ol]	38	-0.124	-0.191	26.746	0.481	89	52	87	54	111	105 original
5402	46 Arabinose	138	[674; Ergosterol (1TMS)]	46	-0.134	0.012	25.948	0.487	90	51	82	59	102	101 original
5371	46 Arabinose	107	9-(Z)-Octadecenoic acid	64	-0.137	-0.359	17.312	0.448	91	50	93	48	52	116 original
5401	46 Arabinose	137	Ergosterol	64	-0.140	-0.222	19.618	0.468	92	49	88	53	71	109 original
5318	46 Arabinose	52	[NA]	64	-0.157	-0.696	31.523	0.674	93	48	114	27	130	21 original
14965	46 Arabinose	43	[548; Leucine (2TBS)]	46	-0.201	-0.365	18.028	0.512	94	47	94	47	59	87 duplicate
5335	46 Arabinose	71	[731; Erythrose (3TMS)]	64	-0.213	-0.283	16.179	0.435	85	46	90	51	48	123 original
10402	46 Arabinose	4	Phosphoric acid	51	-0.227	-0.392	30.734	0.290	96	45	95	46	127	140 duplicate
5388	46 Arabinose	124	[734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	59	-0.241	-0.393	34.017	0.438	97	44	96	45	138	120 original
13048	46 Arabinose	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.257	-0.891	28.544	0.655	98	43	134	7	119	30 duplicate
5394	46 Arabinose	130	Trehalose	63	-0.263	-0.337	25.324	0.379	99	42	92	49	100	133 original
5362	46 Arabinose	98	[697; Ribose-5-phosphate methoxamine (5TMS)]	48	-0.301	-0.748	29.047	0.535	100	41	121	20	121	76 original
5400	46 Arabinose	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.309	-0.496	10.611	0.537	101	40	98	43	11	75 original
5325	46 Arabinose	61	[NA]	64	-0.310	-0.527	19.211	0.517	102	39	101	40	69	84 original
5372	46 Arabinose	108	Octadecanoic acid	64	-0.320	-0.524	21.502	0.404	103	38	100	41	82	131 original
5322	46 Arabinose	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	-0.336	-0.407	19.964	0.389	104	37	97	44	74	132 original
13277	46 Arabinose	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	-0.354	-0.763	30.234	0.565	105	36	122	19	124	67 duplicate
12815	46 Arabinose	23	Homoserine	64	-0.354	-0.802	24.188	0.622	106	35	126	15	94	47 duplicate
5332	46 Arabinose	68	[570; Hypoxanthine (2TMS)]	20	-0.358	-0.921	19.065	0.617	107	34	137	4	67	51 original
5353	46 Arabinose	89	[775; Dopamine (4TMS)]	35	-0.392	-0.888	26.817	0.626	108	33	133	8	112	44 original
5313	46 Arabinose	49	[877; Pyrophosphoric acid (4TMS)]	64	-0.394	-0.590	33.395	0.466	109	32	105	36	134	110 original
14258	46 Arabinose	36	[596; N-Acetylglutamic acid (2TMS)]	64	-0.398	-0.568	26.877	0.427	110	31	104	37	110	128 duplicate
5339	46 Arabinose	75	Lysine	64	-0.403	-0.521	34.801	0.440	111	30	98	42	139	119 original
10807	46 Arabinose	7	Threonine	64	-0.406	-0.544	26.320	0.417	112	29	103	38	106	130 duplicate
15158	46 Arabinose	45	Homocysteine	61	-0.417	-0.594	32.574	0.434	113	28	106	35	132	125 duplicate
10127	46 Arabinose	2	Serine	62	-0.443	-0.595	25.953	0.428	114	27	107	34	103	127 duplicate
5330	46 Arabinose	66	Glyceric acid-3-phosphate	64	-0.456	-0.611	20.789	0.471	115	26	108	33	76	108 original
10940	46 Arabinose	8	Isoleucine	55	-0.461	-0.532	24.041	0.331	116	25	102	39	91	139 duplicate
5359	46 Arabinose	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	-0.466	-0.715	28.811	0.499	117	24	117	24	120	92 original
13723	46 Arabinose	31	[822; Parabanic acid (2TMS)]	64	-0.472	-0.694	24.781	0.541	118	23	113	28	97	73 duplicate
5395	46 Arabinose	131	[626; 5-Methylthioadenosine (3TMS)]	55	-0.476	-0.725	27.560	0.579	119	22	119	22	116	62 original
14047	46 Arabinose	34	Aspartic acid	64	-0.495	-0.825	30.275	0.501	120	21	109	32	125	91 duplicate
5324	46 Arabinose	60	Glycerol-3-phosphate	64	-0.514	-0.654	21.203	0.511	121	19	111	30	78	88 original
5312	46 Arabinose	48	Asparagine	64	-0.518	-0.876	25.977	0.680	122	20	130	11	104	18 original
5331	46 Arabinose	37	Phenylalanine	64	-0.525	-0.689	21.456	0.450	123	18	112	29	81	115 original
14362	46 Arabinose	9	Proline	63	-0.532	-0.725	21.369	0.475	124	17	118	23	80	106 duplicate
11072	46 Arabinose	33	Methionine	64	-0.552	-0.698	23.778	0.514	125	16	110	31	129	129 duplicate
13940	46 Arabinose	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.575	-0.809	26.444	0.510	127	14	115	26	90	85 duplicate
5315	46 Arabinose	30	[815; Ethyl-3(2H)-thiophenone]	64	-0.613	-0.708	30.092	0.435	128	13	116	25	122	124 duplicate
13613	46 Arabinose	55	[612; 4-Aminobutyric acid (2TBS)]	43	-0.628	-0.908	27.768	0.554	129	12	135	6	117	71 original
5319	46 Arabinose	5	Leucine	45	-0.640	-0.780	19.963	0.519	130	11	124	17	73	83 duplicate
10538	46 Arabinose	32	[728; N,N-Dimethyllysine methyl ester]	63	-0.641	-0.819	31.039	0.618	131	10	128	13	128	50 duplicate
13832	46 Arabinose	69	Arginine	60	-0.643	-0.887	26.938	0.643	132	9	132	9	113	36 original
5333	46 Arabinose	3	Ethanolamine	62	-0.654	-0.877	25.890	0.602	133	8	131	10	101	57 duplicate

12458	46 Arabinose	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.660	-0.963	19,732	0.644	134	7	139	2	72	35 duplicate
5323	46 Arabinose	64	Ornithine; Arginine	64	-0.669	-0.736	36,523	0.495	135	6	120	21	140	94 original
5346	46 Arabinose	82	Lysine	39	-0.692	-0.969	25,137	0.691	136	5	140	1	98	12 original
11203	46 Arabinose	10	Glycine	64	-0.700	-0.958	24,112	0.712	137	4	138	3	83	8 duplicate
5341	46 Arabinose	77	[826; beta-[[[5-methyl-2-thienyl)methyl]eneamino- benzeneacetic acid methyl ester]	62	-0.719	-0.837	32,179	0.493	138	3	129	12	131	95 original
14867	46 Arabinose	42	Glutamic acid	60	-0.741	-0.789	33,478	0.485	139	2	125	16	135	102 duplicate
5345	46 Arabinose	81	Tyrosine	64	-0.745	-0.919	33,948	0.661	140	1	136	5	137	25 original
9989	47 [NA]	1	[938; Sulfuric acid (2TMS)]	36	0.584	0.786	5,549	0.862	1	140	1	140	1	1 duplicate
5430	47 [NA]	72	[919; D-Xylopyranose (4TMS)]	63	0.465	0.664	8,399	0.491	2	139	2	139	4	23 original
5445	47 [NA]	80	[772; D-Glucose (5TMS)]	62	0.370	0.542	27,680	0.397	3	138	4	137	120	112 original
5449	47 [NA]	87	[945; beta-D-Glucopyranose (5TMS)]	62	0.358	0.503	33,108	0.459	4	137	7	134	132	44 original
5459	47 [NA]	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	0.354	0.535	14,571	0.457	5	136	5	136	50	51 original
5455	47 [NA]	101	[832; Dopamine (4TMS)]	64	0.350	0.475	10,450	0.414	6	135	9	132	11	98 original
5476	47 [NA]	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	0.347	0.534	18,040	0.508	7	134	6	135	84	15 original
		118	[928; Glucopyranose-6-phosphate (6TMS)]	58	0.304	0.501	9,573	0.457	8	133	8	133	6	52 original
		129	[940; Maltose methoxyamine (6TMS); alpha-D-Glc-(1,4)-D-Glc]	59	0.286	0.311	13,050	0.434	9	132	16	125	32	77 original
5487	47 [NA]	99	[662; Ribose-5-phosphate methoxyamine (6P) (5TMS)]	41	0.280	0.368	11,290	0.598	10	131	11	130	17	4 original
5461	47 [NA]	103	[648; Ethylamine (2TMS)]	63	0.270	0.378	13,976	0.437	11	130	10	131	45	73 original
5463	47 [NA]	105	[705; 2-Ketogluconic acid (5TMS)]	48	0.270	0.351	11,569	0.520	12	129	12	129	19	12 original
5442	47 [NA]	84	Mannitol	62	0.252	0.551	28,711	0.498	13	128	3	138	121	20 original
5450	47 [NA]	92	[680; Glycerol-2-phosphate (4TMS)]	54	0.233	0.258	10,654	0.464	14	127	19	122	12	42 original
5408	47 [NA]	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	0.232	0.314	19,340	0.470	15	126	15	126	93	37 original
12093	47 [NA]	17	[700; 2-methyl-1,2-propanediol (2TMS)]	84	0.218	0.231	17,371	0.445	16	125	24	117	79	65 duplicate
11591	47 [NA]	13	Uracil	64	0.215	0.253	16,162	0.477	17	124	20	121	67	32 duplicate
5412	47 [NA]	54	[NA]	55	0.215	0.155	14,581	0.450	18	123	37	104	51	60 original
5492	47 [NA]	134	Isomaltose	64	0.209	0.243	24,330	0.448	19	122	21	120	115	62 original
5423	47 [NA]	65	[646; 3-Deoxyglucitol (5TMS)]	63	0.208	0.203	16,012	0.491	20	121	29	112	65	25 original
5451	47 [NA]	93	[607; Putrescine (4TMS)]	60	0.206	0.338	16,762	0.420	21	120	13	128	71	93 original
5446	47 [NA]	88	Gluconic acid	64	0.200	0.271	12,944	0.495	22	119	18	123	31	21 original
5411	47 [NA]	53	Glycerol-2-phosphate	64	0.196	0.328	12,858	0.378	23	118	14	127	30	120 original
		57												
5415	47 [NA]	55	[757; 2-Deoxy-pentose-3-yose dimethoxyamine (2TMS)]	55	0.195	0.173	15,346	0.458	24	117	32	109	61	48 original
5414	47 [NA]	56	[829; Orotic acid (3TMS)]	64	0.192	0.241	13,719	0.476	25	116	22	119	41	35 original
15254	47 [NA]	46	Arabinose	64	0.188	0.239	17,974	0.458	26	115	23	118	83	49 duplicate
11969	47 [NA]	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	0.186	0.210	17,584	0.477	27	114	28	113	81	33 duplicate
12933	47 [NA]	24	[725; 2-Ketocotanoic acid (2TMS)]	64	0.180	0.220	30,930	0.466	28	113	26	115	128	41 duplicate
14568	47 [NA]	39	[829; 1-Phenylethanol (1TMS)]	63	0.164	0.156	17,316	0.444	29	112	36	105	78	68 duplicate
12698	47 [NA]	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.157	0.223	13,558	0.422	30	111	25	116	39	87 duplicate
5420	47 [NA]	62	[812; D-Xylofuranose (4TMS)]	64	0.147	0.157	14,539	0.412	31	110	35	106	48	99 original
5478	47 [NA]	120	[945; Uridine (3TMS)]	54	0.124	0.135	12,828	0.447	32	109	39	102	29	64 original
14966	47 [NA]	43	[548; Leucine (2TBS)]	60	0.122	0.152	10,380	0.371	33	108	38	103	9	126 duplicate
5407	47 [NA]	49	[977; Fructose-6-phosphate methoxyamine (6TMS)]	64	0.108	0.218	20,480	0.421	34	107	27	114	88	90 original
5485	47 [NA]	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.104	0.300	7,767	0.499	35	106	17	124	3	18 original
11334	47 [NA]	86	[793; D-Galactono-1,4-lactone (4TMS)]	61	0.104	0.168	22,664	0.451	36	105	33	108	107	57 original
13503	47 [NA]	11	Succinic acid	64	0.100	0.075	10,794	0.421	37	104	44	97	13	91 duplicate
5486	47 [NA]	29	Erythritol	64	0.099	0.131	10,157	0.480	38	103	40	101	7	30 duplicate
		128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.075	0.042	10,444	0.498	39	102	48	93	10	19 original
5440	47 [NA]	82	Lysine	39	0.074	0.189	18,067	0.484	40	101	31	110	86	28 original

5421	47 [NA]	63	Glutamine	52	0.071	-0.084	18,059	0.458	41	100	69	72	85	46 original
14466	47 [NA]	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.065	-0.054	10,908	0.444	42	99	42	99	15	66 duplicate
13049	47 [NA]	25	[708; 2,5-Diaminovalerolactam (2TMS)]	48	0.060	-0.054	17,123	0.552	43	98	68	73	76	8 duplicate
5428	47 [NA]	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	0.046	-0.014	19,451	0.317	44	97	62	79	94	136 original
5483	47 [NA]	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	0.044	0.161	30,926	0.372	45	98	34	107	127	125 original
13164	47 [NA]	26	Citramalic acid	64	0.037	0.033	16,545	0.406	46	95	51	80	69	102 duplicate
11463	47 [NA]	12	Glyceric acid	63	0.033	0.034	13,923	0.458	47	94	50	81	44	47 duplicate
11718	47 [NA]	14	Fumaric acid	64	0.029	0.062	12,426	0.430	48	93	45	96	25	80 duplicate
10539	47 [NA]	5	Leucine	45	0.022	0.191	10,290	0.429	49	92	30	111	8	81 duplicate
10674	47 [NA]	6	Glycerol	64	0.020	0.113	40,578	0.399	50	91	41	100	140	109 duplicate
14769	47 [NA]	41	[638; Proline (2TMS)]	64	0.017	0.021	14,693	0.426	51	90	54	87	53	84 duplicate
5448	47 [NA]	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	64	0.008	0.052	10,819	0.374	52	89	47	94	14	124 original
5475	47 [NA]	117	[724; Glycerol (3TMS)]	56	0.004	-0.098	13,080	0.531	53	88	73	68	33	10 original
12579	47 [NA]	21	[678; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	64	0.000	-0.024	17,048	0.398	54	87	65	76	75	110 duplicate
5464	47 [NA]	108	[733; Threitol (4TMS)]	62	-0.003	-0.027	14,556	0.534	55	86	66	75	49	9 original
5447	47 [NA]	89	[775; Dopamine (4TMS)]	35	-0.018	-0.015	16,775	0.420	56	85	64	77	72	94 original
12459	47 [NA]	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.019	0.012	14,532	0.329	57	84	58	85	47	135 duplicate
10403	47 [NA]	4	Phosphoric acid	51	-0.020	-0.263	34,100	0.365	58	83	99	42	134	127 duplicate
5468	47 [NA]	110	[715; Erythritol (4TMS)]	54	-0.022	-0.005	15,309	0.614	59	82	58	83	60	3 original
11844	47 [NA]	15	Alanine	64	-0.025	-0.020	18,771	0.409	60	81	55	86	91	100 duplicate
5436	47 [NA]	78	Mannose	62	-0.025	-0.011	14,987	0.457	61	80	59	82	55	50 original
5470	47 [NA]	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (8TMS)]	63	-0.028	-0.105	18,222	0.453	62	79	74	67	89	56 original
5479	47 [NA]	121	[657; Erythritol (4TMS)]	55	-0.036	-0.151	16,666	0.486	63	78	79	62	70	27 original
5480	47 [NA]	122	[644; Erythritol (4TMS)]	52	-0.038	-0.052	18,170	0.573	64	77	67	74	87	6 original
13278	47 [NA]	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	-0.042	-0.133	20,521	0.386	65	76	76	65	99	118 duplicate
5454	47 [NA]	96	myo-Inositol	49	-0.043	-0.091	18,931	0.317	66	75	71	70	92	137 original
13391	47 [NA]	28	Malic acid	64	-0.047	0.001	11,639	0.456	67	74	57	84	20	54 duplicate
5434	47 [NA]	76	Fructose	64	-0.051	0.057	25,438	0.448	68	73	46	95	118	63 original
5473	47 [NA]	115	Glucose-6-phosphate	62	-0.051	-0.013	24,743	0.477	69	72	60	81	116	34 original
5489	47 [NA]	131	[626; 5-Methylthioadenosine (3TMS)]	55	-0.053	0.083	17,741	0.443	70	71	43	98	82	70 original
15159	47 [NA]	45	Homocysteine	61	-0.056	0.022	22,891	0.387	71	70	53	88	108	116 duplicate
14154	47 [NA]	35	Pyroglutamic acid	64	-0.061	0.025	40,224	0.396	72	69	52	89	138	113 duplicate
14669	47 [NA]	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.070	-0.136	33,602	0.499	73	68	77	64	133	17 duplicate
5497	47 [NA]	139	[700; Ergosta-5,7-dien-3-ol]	38	-0.073	-0.106	18,878	0.359	74	67	75	66	74	130 original
12338	47 [NA]	19	Alanine [BP] (3TMS)	64	-0.073	-0.013	13,900	0.449	75	66	61	80	43	61 duplicate
5493	47 [NA]	135	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	-0.080	-0.219	13,526	0.425	76	65	91	50	38	85 original
5410	47 [NA]	52	[NA]	46	-0.094	-0.084	21,554	0.469	77	64	70	71	103	39 original
5490	47 [NA]	132	[895; Isomaltose methoxyamine (8TMS)]	42	-0.094	0.041	17,234	0.504	78	63	49	92	77	16 original
5413	47 [NA]	55	[612; 4-Aminobutyric acid (2TBS)]	43	-0.101	-0.147	21,220	0.308	79	62	78	63	101	138 original
5458	47 [NA]	100	[857; Mannitol (6TMS)]	64	-0.105	-0.240	12,206	0.450	80	61	95	46	24	59 original
5437	47 [NA]	79	Glucose	64	-0.109	-0.015	34,212	0.432	81	60	63	78	135	78 original
12216	47 [NA]	18	[590; 1-Acetyl-2-thioidantoin]	64	-0.121	-0.257	11,873	0.416	82	59	98	43	22	97 duplicate
5465	47 [NA]	107	9-(Z)-Octadecenoic acid	64	-0.129	-0.157	15,597	0.376	83	58	80	61	62	121 original
5494	47 [NA]	138	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.132	-0.373	6,510	0.480	84	57	111	30	2	29 original
5432	47 [NA]	74	[912; Tetradecanoic acid (1TMS)]	64	-0.134	-0.286	16,035	0.491	85	56	102	39	66	24 original
5431	47 [NA]	73	[708; Glucose methoxyamine (5TMS)]	57	-0.139	-0.205	15,062	0.401	86	55	88	53	55	105 original
5477	47 [NA]	119	[931; myo-Inositol-2-phosphate (7TMS)]	64	-0.143	-0.180	12,698	0.349	87	54	84	57	28	132 original
5408	47 [NA]	95	Asparagine	64	-0.145	-0.173	15,682	0.400	88	53	83	58	64	108 original
5453	47 [NA]	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	-0.149	-0.206	22,400	0.302	89	52	89	52	105	139 original

5422	47 [NA]	64 [789; Tyramine (3TMS)]	63 -0.150	-0.253	10.952	0.334	90	51	97	44	16	134 original
5460	47 [NA]	102 [804; Galactose methoxymine (5TMS)]	64 -0.151	-0.336	11.962	0.456	91	50	106	35	23	53 original
14048	47 [NA]	34 Aspartic acid	64 -0.154	-0.189	32.447	0.366	92	48	86	55	131	117 duplicate
5468	47 [NA]	108 Octadecanoic acid	64 -0.154	-0.232	12.518	0.421	93	49	94	47	26	92 original
5488	47 [NA]	130 Trehalose	63 -0.168	-0.182	29.380	0.420	94	47	85	56	123	95 original
5481	47 [NA]	123 [945; Galactofuranose-6-phosphate (7TMS)]	64 -0.173	-0.207	13.280	0.469	95	46	90	51	36	38 original
5498	47 [NA]	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49 -0.182	-0.273	15.681	0.361	96	45	100	41	63	128 original
12816	47 [NA]	23 Homoserine	64 -0.188	-0.161	14.678	0.444	97	44	81	60	52	67 duplicate
5474	47 [NA]	116 [882; Pseudouridine (5TMS)]	30 -0.195	-0.400	11.515	0.459	98	43	117	24	18	45 original
5427	47 [NA]	69 Arginine	60 -0.200	-0.219	22.934	0.466	99	42	92	49	109	40 original
5462	47 [NA]	104 [785; Erythritol (4TMS)]	63 -0.201	-0.242	13.136	0.450	100	41	96	45	34	58 original
5419	47 [NA]	114 Fructose-6-phosphate	64 -0.204	-0.339	11.664	0.375	101	40	107	34	21	123 original
5472	47 [NA]	85 [529; Methylenic acid (4TMS)]	53 -0.209	-0.168	13.138	0.569	102	39	82	59	35	5 original
5443	47 [NA]	113 Galactose-6-phosphate	48 -0.215	-0.324	9.044	0.388	103	38	105	36	5	115 original
5471	47 [NA]	126 [559; Erythritol (4TMS)]	62 -0.215	-0.092	13.477	0.513	104	37	72	69	37	14 original
13833	47 [NA]	32 [729; N,N-Dimethyllysine methyl ester]	63 -0.216	-0.353	20.594	0.492	105	36	109	32	100	22 duplicate
15063	47 [NA]	44 [910; 2-Ketogluconic acid methoxymine (4TMS)]	50 -0.224	-0.430	15.158	0.571	106	35	121	20	58	7 duplicate
		58 [636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64 -0.225	-0.385	18.481	0.435	107	34	113	28	90	74 original
5416	47 [NA]	33 Methionine	64 -0.238	-0.223	15.184	0.392	108	33	93	48	59	114 duplicate
13941	47 [NA]	10 Glycine	60 -0.246	-0.295	20.464	0.434	109	32	103	38	97	76 duplicate
11204	47 [NA]	42 Glutamic acid	60 -0.253	-0.381	31.533	0.384	110	31	110	31	130	119 duplicate
14868	47 [NA]	141 Lanosta-8,24-dien-3-beta-ol	61 -0.259	-0.350	16.820	0.375	111	30	108	33	73	122 original
5499	47 [NA]	126 [559; Erythritol (4TMS)]	45 -0.261	-0.457	13.605	0.632	112	29	123	18	40	2 original
5484	47 [NA]	8 Isolaudine	55 -0.263	-0.429	22.418	0.356	113	28	120	21	108	131 duplicate
10941	47 [NA]	30 [815; Ethyl-3-(2H)-thiophenone]	64 -0.264	-0.277	30.349	0.400	114	27	101	40	125	107 duplicate
13614	47 [NA]	77 [826; beta-[[[5-methyl-2-thienyl)methyl]eneamino- benzeneacetic acid methyl ester]	62 -0.266	-0.423	31.379	0.403	115	26	119	22	129	103 original
5435	47 [NA]	2 Serine	62 -0.267	-0.492	23.111	0.422	116	25	130	11	110	89 duplicate
10128	47 [NA]	98 [697; Ribose-5-phosphate methoxymine (5TMS)]	48 -0.270	-0.204	21.427	0.428	117	24	87	54	102	82 original
5456	47 [NA]	75 Lysine	64 -0.272	-0.480	39.331	0.431	118	23	127	14	137	79 original
5433	47 [NA]	59 Ornithine; Arginine	64 -0.280	-0.381	40.428	0.399	119	22	112	29	139	108 original
5417	47 [NA]	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44 -0.288	-0.318	20.372	0.339	120	21	104	37	96	133 original
5409	47 [NA]	31 [622; Parabanic acid (2TMS)]	64 -0.290	-0.396	15.110	0.401	121	19	115	26	57	104 duplicate
13724	47 [NA]	133 [855; Squalene]	64 -0.290	-0.417	13.761	0.397	122	20	118	23	42	111 original
5491	47 [NA]	111 [583; Erythritol (4TMS)]	42 -0.301	-0.503	20.100	0.443	123	18	132	9	95	69 original
5469	47 [NA]	124 [734; 1-Monooldeoylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	59 -0.320	-0.386	25.137	0.419	124	17	114	27	117	96 original
5482	47 [NA]	9 Proline	63 -0.321	-0.502	30.380	0.424	125	16	131	10	126	86 duplicate
11073	47 [NA]	66 Glyceric acid-3-phosphate	64 -0.325	-0.523	12.541	0.455	126	15	134	7	27	55 original
5424	47 [NA]	81 Tyrosine	64 -0.332	-0.484	34.828	0.524	127	14	128	13	136	11 original
5439	47 [NA]	137 Ergosterol	64 -0.334	-0.438	18.188	0.360	128	13	122	19	88	129 original
5495	47 [NA]	109 Octadecanoic acid	64 -0.339	-0.478	25.482	0.486	129	12	125	16	119	26 original
5467	47 [NA]	94 Hexadecanoic acid	64 -0.346	-0.480	23.559	0.479	130	11	126	15	113	31 original
5452	47 [NA]	36 [596; N-Acetylglutamic acid (2TMS)]	64 -0.354	-0.560	29.370	0.463	131	10	135	6	122	43 duplicate
14259	47 [NA]	3 Ethanolamine	62 -0.370	-0.468	16.214	0.439	132	9	124	17	68	72 duplicate
10266	47 [NA]	138 [674; Ergosterol (1TMS)]	46 -0.397	-0.516	17.531	0.440	133	8	133	8	80	71 original
5496	47 [NA]	68 [570; Hypoxanthine (2TMS)]	20 -0.411	-0.396	14.870	0.240	134	7	116	25	54	140 original
5426	47 [NA]	83 Sorbitol	58 -0.429	-0.490	23.325	0.408	135	6	129	12	112	101 original
5441	47 [NA]	37 Phenylalanine	64 -0.443	-0.588	23.116	0.422	136	5	137	4	111	88 duplicate
14363	47 [NA]	60 Glyceral-3-phosphate	64 -0.448	-0.607	22.378	0.471	137	4	138	3	104	36 original

10808	47 [NA]	7 Threonine	64 -0.457	-0.569	30.018	0.426	138	3	136	5	124	83 duplicate
5425	47 [NA]	67 Citric acid	64 -0.470	-0.610	23.832	0.435	139	2	139	2	114	75 original
5429	47 [NA]	71 [731; Erythrose (3TMS)]	64 -0.493	-0.672	14.309	0.519	140	1	140	1	46	13 original
5519	48 Asparagine	68 [570; Hypoxanthine (2TMS)]	20 0.842	0.958	17.879	0.639	1	140	1	140	68	15 original
5502	48 Asparagine	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44 0.751	0.844	21.331	0.580	2	139	7	134	99	42 original
5506	48 Asparagine	55 [612; 4-Aminobutyric acid (2TBS)]	43 0.714	0.849	23.193	0.619	3	138	6	135	108	22 original
11205	48 Asparagine	10 Glycine	64 0.887	0.892	14.434	0.669	4	137	4	137	37	7 duplicate
5533	48 Asparagine	82 Lysine	39 0.676	0.933	8.048	0.675	5	136	2	139	3	4 original
5540	48 Asparagine	89 [775; Dopamine (4TMS)]	35 0.661	0.894	12.539	0.602	6	135	3	138	21	33 original
5532	48 Asparagine	81 Tyrosine	64 0.654	0.803	29.744	0.636	7	134	11	130	125	19 original
10540	48 Asparagine	5 Leucine	45 0.653	0.680	10.162	0.487	8	133	20	121	11	93 duplicate
5582	48 Asparagine	131 [626; 5-Methylthioadenosine (3TMS)]	55 0.636	0.797	16.506	0.598	9	132	12	129	57	36 original
		77 [826; beta-[[[5-methyl-2-thienyl)methyl]eneamino- benzeneacetic acid methyl ester]	62 0.634	0.736	24.881	0.526	10	131	15	126	116	73 original
5528	48 Asparagine	3 Ethanolamine	62 0.621	0.830	10.436	0.600	11	130	8	133	12	34 duplicate
10267	48 Asparagine	42 Glutamic acid	60 0.620	0.652	24.452	0.500	12	129	23	118	113	83 duplicate
14869	48 Asparagine	69 Arginine	60 0.619	0.822	15.481	0.614	13	128	9	132	47	24 original
5520	48 Asparagine	30 [815; Ethyl-3(2H)-thiophenone]	64 0.581	0.607	26.245	0.428	14	127	30	111	119	118 duplicate
13615	48 Asparagine											
12460	48 Asparagine	20 [619; 2-(3',4'-Bishydroxyphenyl)-2-oxethylamine (4TMS)]	31 0.561	0.680	17.273	0.676	15	126	5	136	63	3 duplicate
13050	48 Asparagine	25 [709; 2,5-Diaminovalerolactam (2TMS)]	48 0.560	0.789	9.168	0.608	16	125	13	128	8	31 duplicate
5510	48 Asparagine	59 Ornithine; Arginine	64 0.560	0.673	38.072	0.503	17	124	21	120	138	82 original
13725	48 Asparagine	31 [622; Parabenic acid (2TMS)]	64 0.534	0.684	11.609	0.500	18	123	19	122	20	84 duplicate
5546	48 Asparagine	95 [770; 3,4,6-Trisubstitutedphenylmethanolamine (5TMS)]	50 0.530	0.718	21.077	0.563	19	122	17	124	95	55 original
13942	48 Asparagine	33 Methionine	64 0.528	0.595	8.963	0.484	20	121	31	110	7	95 duplicate
15160	48 Asparagine	45 Homocysteine	61 0.525	0.686	22.308	0.459	21	120	18	123	105	110 duplicate
5503	48 Asparagine	52 [NA]	46 0.511	0.722	18.452	0.646	22	119	16	125	74	13 original
14384	48 Asparagine	37 Phenylalanine	64 0.505	0.635	20.917	0.493	23	118	29	112	94	90 duplicate
10942	48 Asparagine	8 Isoleucine	55 0.495	0.394	15.662	0.351	24	117	40	101	49	136 duplicate
5512	48 Asparagine	61 [NA]	64 0.494	0.643	8.681	0.531	25	116	27	114	6	72 original
12817	48 Asparagine	23 Homoserine	64 0.485	0.749	7.069	0.574	26	115	14	127	2	48 duplicate
13834	48 Asparagine	32 [729; N,N-Dimethyllysine methyl ester]	63 0.482	0.670	13.112	0.564	27	114	22	119	28	54 duplicate
5500	48 Asparagine	49 [877; Pyrophosphoric acid (4TMS)]	64 0.481	0.645	18.653	0.478	28	113	26	115	76	100 original
14049	48 Asparagine	34 Aspartic acid	64 0.479	0.577	29.837	0.475	29	112	32	109	126	103 duplicate
5518	48 Asparagine	67 Citric acid	64 0.474	0.637	22.122	0.494	30	111	28	113	103	89 original
5514	48 Asparagine	63 Glutamine	52 0.460	0.604	10.113	0.654	31	110	10	131	9	11 original
11074	48 Asparagine	9 Proline	63 0.448	0.538	23.837	0.442	32	109	36	105	111	111 duplicate
5511	48 Asparagine	60 Glycerol-3-phosphate	64 0.423	0.538	19.542	0.482	34	107	34	107	86	79 original
5549	48 Asparagine	98 [697; Ribose-5-phosphate methoxymine (5TMS)]	48 0.397	0.652	18.977	0.510	33	108	24	117	79	97 original
14867	48 Asparagine	43 [548; Leucine (2TBS)]	60 0.350	0.539	8.569	0.514	35	106	33	108	4	76 duplicate
5517	48 Asparagine	66 Glycic acid-3-phosphate	64 0.339	0.488	10.135	0.475	36	105	35	106	10	102 original
13279	48 Asparagine	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53 0.331	0.645	17.338	0.538	37	104	25	116	64	67 duplicate
10129	48 Asparagine	2 Serine	62 0.310	0.404	16.290	0.437	38	103	39	102	54	114 duplicate
10809	48 Asparagine	7 Threonine	64 0.307	0.417	28.236	0.408	39	102	38	103	122	124 duplicate
5559	48 Asparagine	108 Octadecanoic acid	64 0.229	0.423	10.445	0.397	40	101	37	104	13	129 original
14260	48 Asparagine	36 [596; N-Acetylglutamic acid (2TMS)]	64 0.211	0.358	26.499	0.432	41	100	41	100	120	116 duplicate
5526	48 Asparagine	75 Lysine	64 0.206	0.346	37.406	0.424	42	99	42	99	137	119 original
5522	48 Asparagine	71 [731; Erythrose (3TMS)]	64 0.162	0.203	12.694	0.438	43	98	48	93	22	113 original
5587	48 Asparagine	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17 0.147	0.338	5.263	0.403	44	97	43	98	1	126 original
5558	48 Asparagine	107 9-(Z)-Octadecanoic acid	64 0.113	0.308	14.150	0.403	45	96	44	97	36	127 original



5575	48 Asparagine	124 [734; 1-Monodeoxyglycerol (2TMS); 1-	59 0.099	0.250	24.713	0.398	46	95	46	95	114	132 original
5581	48 Asparagine	Mono-hexadecenoxyglycerol (1TMS)]	63 0.095	0.146	28.486	0.334	47	94	51	90	123	138 original
5589	48 Asparagine	130 Trehalose	64 0.090	0.267	15.283	0.408	48	93	45	96	45	125 original
5570	48 Asparagine	58 [636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane	64 0.081	0.244	10.740	0.478	49	92	47	94	14	99 original
5544	48 Asparagine	(1TMS)]	60 0.068	-0.051	19.310	0.441	50	91	58	83	82	112 original
5504	48 Asparagine	119 [931; myo-Inositol-2-phosphate (7TMS)]	64 0.052	0.154	14.144	0.397	51	90	50	91	35	130 original
5588	48 Asparagine	53 Glycerol-2-phosphate	64 0.031	0.143	14.784	0.419	52	89	52	89	42	121 original
5541	48 Asparagine	137 Ergosterol	64 0.028	0.137	10.765	0.434	53	88	54	87	15	115 original
10404	48 Asparagine	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	51 0.010	0.167	30.393	0.326	54	87	49	92	129	140 duplicate
5523	48 Asparagine	4 Phosphoric acid	63 0.008	0.039	13.352	0.330	55	86	55	86	30	139 original
5535	48 Asparagine	72 [919; D-Xylopyranose (4TMS)]	62 0.002	-0.235	31.284	0.464	56	85	64	77	130	105 original
5592	48 Asparagine	84 Mannitol	61 -0.061	-0.039	17.366	0.485	57	84	57	84	65	94 original
5515	48 Asparagine	141 Lanosta-8,24-dien-3-beta-ol	63 -0.078	-0.299	11.530	0.424	58	83	67	74	19	120 original
5545	48 Asparagine	64 [789; Tyramine (3TMS)]	64 -0.090	-0.309	22.554	0.459	59	82	69	72	108	108 original
9990	48 Asparagine	94 Hexadecanoic acid	38 -0.098	-0.384	10.912	0.568	60	81	72	69	16	52 duplicate
5589	48 Asparagine	1 [938; Sulfuric acid (2TMS)]	48 -0.109	-0.177	18.308	0.429	61	80	61	80	72	117 original
5560	48 Asparagine	138 [674; Ergosterol (1TMS)]	64 -0.111	-0.394	24.790	0.459	62	79	73	68	115	109 original
11845	48 Asparagine	109 Octadecanoic acid	64 -0.128	-0.465	20.278	0.635	63	78	78	65	90	20 duplicate
5534	48 Asparagine	83 Sorbitol	58 -0.139	0.138	19.483	0.365	64	77	53	88	85	134 original
15349	48 Asparagine	47 [NA]	64 -0.145	-0.173	15.682	0.400	65	76	60	81	50	128 duplicate
5590	48 Asparagine	139 [700; Ergosta-5,7-dien-3-ol]	38 -0.158	0.014	19.071	0.416	66	74	56	85	80	122 original
5578	48 Asparagine	127 [777; Fructose-6-phosphate methoxamine (6TMS)]	39 -0.158	-0.276	8.678	0.569	67	75	65	76	5	50 original
5584	48 Asparagine	133 [855; Squalene]	64 -0.171	-0.140	12.821	0.368	68	73	59	82	24	133 original
5562	48 Asparagine	111 [583; Erythritol (4TMS)]	42 -0.171	-0.298	18.823	0.358	69	72	66	75	77	135 original
5591	48 Asparagine	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49 -0.201	-0.207	18.860	0.475	70	71	62	78	78	101 original
5550	48 Asparagine	99 [682; Ribose-5-phosphate methoxamine (BP) (5TMS)]	41 -0.217	-0.741	14.832	0.613	71	70	104	37	41	25 original
5586	48 Asparagine	135	64 -0.217	-0.372	13.544	0.460	72	69	71	70	32	107 original
5548	48 Asparagine	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	52 -0.238	-0.547	25.709	0.549	73	68	82	59	117	61 original
5530	48 Asparagine	79 Glucose	64 -0.242	-0.680	35.257	0.611	74	67	95	46	135	28 original
5556	48 Asparagine	105 [705; 2-Ketogluconic acid (5TMS)]	48 -0.257	-0.396	16.247	0.533	75	66	74	67	53	71 original
5547	48 Asparagine	96 myo-Inositol	49 -0.262	-0.301	22.291	0.338	76	65	68	73	104	137 original
5569	48 Asparagine	118 [928; Glucopyranose-6-phosphate (6TMS)]	58 -0.266	-0.428	14.917	0.465	77	64	75	66	43	104 original
5579	48 Asparagine	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45 -0.275	-0.504	12.695	0.561	78	63	79	62	23	57 original
5563	48 Asparagine	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63 -0.287	-0.509	19.659	0.488	79	62	80	61	89	92 original
5577	48 Asparagine	126 [559; Erythritol (4TMS)]	45 -0.297	-0.563	11.121	0.586	80	61	87	54	17	41 original
5567	48 Asparagine	116 [882; Pseudouridine (5TMS)]	30 -0.315	-0.232	13.389	0.396	81	60	63	78	31	131 original
5542	48 Asparagine	91 [766; beta-D-Methylglucopyranoside (4TMS)]	64 -0.320	-0.473	23.768	0.489	82	59	77	64	110	91 original
5536	48 Asparagine	85 [529; Methylcitric acid (4TMS)]	64 -0.326	-0.532	11.343	0.461	83	58	81	60	18	106 original
5553	48 Asparagine	102 [904; Galactose methoxamine (5TMS)]	64 -0.329	-0.476	12.973	0.494	84	57	78	63	25	88 original
5574	48 Asparagine	123 [945; Galactofuranose-6-phosphate (7TMS)]	64 -0.337	-0.626	14.539	0.554	85	56	90	51	39	59 original
5564	48 Asparagine	113 Galactose-6-phosphate	62 -0.338	-0.767	17.222	0.554	86	55	112	29	82	60 original
5551	48 Asparagine	100 [857; Mannitol (6TMS)]	64 -0.339	-0.548	13.258	0.513	87	54	83	58	29	77 original
5555	48 Asparagine	104 [795; Erythritol (4TMS)]	63 -0.343	-0.557	15.109	0.510	88	53	85	56	44	78 original
12217	48 Asparagine	18 [590; 1-Acetyl-2-thiohydantoin]	64 -0.343	-0.555	13.043	0.416	89	52	84	57	27	123 duplicate
11464	48 Asparagine	12 Glyceric acid	63 -0.347	-0.652	16.394	0.547	90	51	92	49	55	62 duplicate
15064	48 Asparagine	44 [910; 2-Ketogluconic acid methoxamine (4TMS)]	50 -0.355	-0.675	15.604	0.576	91	50	94	47	48	45 duplicate
10675	48 Asparagine	6 Glycerol	64 -0.357	-0.747	40.845	0.542	92	49	108	35	140	64 duplicate
5525	48 Asparagine	74 [912; Tetradecanoic acid (1TMS)]	64 -0.358	-0.579	18.238	0.480	93	48	88	53	71	98 original

5565	48 Asparagine	114	Fructose-6-phosphate	53	-0.379	-0.792	16.207	0.561	84	47	118	23	52	58 original
5571	48 Asparagine	120	[945; Uridine (3TMS)]	54	-0.399	-0.317	14.537	0.577	95	46	70	71	38	44 original
14770	48 Asparagine	41	[639; Proline (2TMS)]	64	-0.400	-0.639	16.711	0.484	96	45	91	50	58	96 duplicate
5552	48 Asparagine	101	[832; Dopamine (4TMS)]	64	-0.402	-0.560	18.193	0.504	97	44	86	55	70	81 original
13504	48 Asparagine	29	Erythritol	64	-0.405	-0.744	13.010	0.608	98	43	105	36	26	30 duplicate
5543	48 Asparagine	92	[680; Glycerol-2-phosphate (4TMS)]	54	-0.416	-0.749	15.740	0.534	99	42	108	33	51	69 original
5573	48 Asparagine	122	[644; Erythritol (4TMS)]	52	-0.418	-0.729	19.255	0.557	100	41	100	41	81	58 original
5505	48 Asparagine	54	[NA]	55	-0.421	-0.738	17.501	0.570	101	40	103	38	66	49 original
5561	48 Asparagine	110	[715; Erythritol (4TMS)]	54	-0.424	-0.773	18.643	0.600	102	39	114	27	75	35 original
12699	48 Asparagine	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	-0.428	-0.707	17.526	0.568	103	38	99	42	67	51 duplicate
14569	48 Asparagine	39	[829; 1-Phenylethanol (1TMS)]	63	-0.432	-0.810	23.469	0.610	104	37	123	18	109	29 duplicate
5554	48 Asparagine	103	[648; Ethylamine (2TMS)]	63	-0.435	-0.817	21.763	0.519	105	36	89	52	101	74 original
5568	48 Asparagine	117	[724; Glycerol (3TMS)]	56	-0.436	-0.704	16.456	0.516	106	35	98	43	56	75 original
5572	48 Asparagine	121	[657; Erythritol (4TMS)]	55	-0.440	-0.698	17.998	0.538	107	34	87	44	69	68 original
5508	48 Asparagine	757	[2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55	-0.441	-0.825	21.980	0.631	108	33	124	17	102	21 original
14467	48 Asparagine	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.450	-0.790	14.587	0.611	109	32	117	24	40	27 duplicate
12094	48 Asparagine	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	-0.452	-0.771	21.326	0.596	110	31	113	28	98	37 duplicate
12339	48 Asparagine	19	Alanine (BP) (3TMS)	64	-0.460	-0.764	17.118	0.566	111	30	111	30	61	53 duplicate
11335	48 Asparagine	11	Succinic acid	64	-0.461	-0.748	13.630	0.574	112	28	107	34	33	46 duplicate
12580	48 Asparagine	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	-0.464	-0.684	18.354	0.506	113	28	96	45	73	80 duplicate
5580	48 Asparagine	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	-0.468	-0.848	21.154	0.669	114	27	132	9	96	6 original
5524	48 Asparagine	73	[708; Glucose methoxyamine (5TMS)]	57	-0.479	-0.737	19.398	0.533	115	26	102	39	83	70 original
11970	48 Asparagine	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	-0.479	-0.796	20.779	0.639	116	25	120	21	92	16 duplicate
5566	48 Asparagine	115	Glucose-6-phosphate	62	-0.481	-0.835	26.629	0.592	117	24	131	10	121	39 original
5531	48 Asparagine	80	[772; D-Glucose (5TMS)]	62	-0.482	-0.759	32.642	0.497	118	23	110	31	131	87 original
12934	48 Asparagine	24	[725; 2-Ketocacetic acid (2TMS)]	64	-0.487	-0.832	33.093	0.665	119	22	129	12	132	9 duplicate
5529	48 Asparagine	78	Mannose	62	-0.488	-0.788	20.296	0.543	120	21	122	19	91	63 original
14670	48 Asparagine	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.489	-0.750	33.327	0.574	121	20	109	32	133	47 duplicate
5539	48 Asparagine	88	Gluconic acid	64	-0.490	-0.785	19.462	0.662	122	19	119	22	84	10 original
13165	48 Asparagine	26	Citramalic acid	64	-0.499	-0.730	17.053	0.497	123	18	101	40	60	86 duplicate
13392	48 Asparagine	58	Malic acid	64	-0.501	-0.785	13.873	0.577	124	17	115	26	34	43 duplicate
5507	48 Asparagine	64	[829; Oxalic acid (3TMS)]	64	-0.508	-0.862	21.425	0.667	125	16	135	6	100	8 original
5501	48 Asparagine	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	-0.508	-0.797	22.660	0.594	126	15	121	20	107	38 original
13255	48 Asparagine	48	Arabinose	64	-0.514	-0.876	25.977	0.680	127	14	138	3	118	2 duplicate
5583	48 Asparagine	132	[895; Isomaltose methoxyamine (8TMS)]	42	-0.515	-0.835	19.589	0.541	128	13	130	11	87	65 original
5537	48 Asparagine	86	[793; D-Galactono-1,4-lactone (4TMS)]	57	-0.516	-0.887	29.921	0.650	129	12	140	1	127	12 original
5521	48 Asparagine	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	63	-0.517	-0.858	24.048	0.498	130	11	93	48	93	85 original
5516	48 Asparagine	65	[646; 3-Deoxyglucitol (5TMS)]	64	-0.517	-0.787	15.476	0.589	132	9	116	25	46	40 duplicate
11719	48 Asparagine	14	Fumaric acid	64	-0.525	-0.862	30.038	0.671	133	8	137	4	128	5 original
5585	48 Asparagine	35	Pyrogulamic acid	64	-0.527	-0.862	40.722	0.636	134	7	136	5	139	18 duplicate
14155	48 Asparagine	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	-0.530	-0.859	34.057	0.608	135	6	134	7	134	32 original
5576	48 Asparagine	76	Fructose	64	-0.531	-0.884	29.169	0.618	136	5	139	2	124	23 original
5527	48 Asparagine	87	[945; beta-D-Glucopyranose (5TMS)]	62	-0.535	-0.826	36.980	0.540	137	4	126	15	136	66 original
5538	48 Asparagine	106	[733; Threitol (4TMS)]	62	-0.546	-0.826	19.638	0.644	138	3	125	16	88	14 original
5557	48 Asparagine	62	[812; D-Xylofuranose (4TMS)]	64	-0.550	-0.831	16.758	0.612	139	2	128	13	59	26 original
5513	48 Asparagine	13	Uracil	64	-0.563	-0.827	21.282	0.639	140	1	127	14	97	17 duplicate
11592	48 Asparagine	82	Lysine	39	0.714	0.875	22.347	0.529	1	140	1	140	65	2 original
5625	49 [877; Pyrophosphoric ac	89	[775; Dopamine (4TMS)]	35	0.624	0.739	9.589	0.451	2	139	5	136	4	56 original

10541	49 [877; Pyrophosphoric ac	5	Leucine	45	0.604	0.745	10,713	0.496	3	138	4	137	10	21 duplicate
5674	49 [877; Pyrophosphoric ac	131	[826; 5-Methylthioadenosine (3TMS)]	55	0.580	0.760	7,316	0.493	4	137	2	139	2	23 original
5598	49 [877; Pyrophosphoric ac	55	[612; 4-Aminobutyric acid (2TBS)]	43	0.553	0.696	10,450	0.441	5	136	7	134	7	65 original
5638	49 [877; Pyrophosphoric ac	95	[770; 3,4,8-Trisubstitutedphenylethanolamine (5TMS)]	50	0.551	0.700	9,439	0.502	6	135	6	135	3	16 original
5612	49 [877; Pyrophosphoric ac	69	Arginine	60	0.537	0.623	32,002	0.499	7	134	11	130	101	17 original
12461	49 [877; Pyrophosphoric ac	20	[619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	31	0.535	0.760	8,953	0.513	8	133	3	138	1	8 duplicate
15161	49 [877; Pyrophosphoric ac	45	Homocysteine	61	0.486	0.630	10,493	0.408	9	132	9	132	9	90 duplicate
14870	49 [877; Pyrophosphoric ac	42	Glutamic acid	60	0.485	0.435	40,195	0.365	10	131	22	119	118	114 duplicate
13051	49 [877; Pyrophosphoric ac	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	0.482	0.479	15,047	0.455	11	130	17	124	28	50 duplicate
15443	49 [877; Pyrophosphoric ac	48	Asparagine	64	0.481	0.645	18,653	0.478	12	129	8	133	48	32 duplicate
11206	49 [877; Pyrophosphoric ac	10	Glycine	64	0.459	0.628	31,065	0.483	13	128	10	131	98	28 duplicate
5606	49 [877; Pyrophosphoric ac	63	Glutamine	52	0.454	0.603	14,732	0.413	14	127	12	129	26	86 original
13943	49 [877; Pyrophosphoric ac	33	Methionine	64	0.424	0.445	20,056	0.378	15	126	21	120	55	103 duplicate
5620	49 [877; Pyrophosphoric ac	77	[826; beta-[(5-methyl-2-thienyl)methyl]eneamino-benzeneacetic acid methyl ester]	62	0.419	0.421	41,801	0.433	16	125	23	118	121	72 original
13616	49 [877; Pyrophosphoric ac	30	[815; Ethyl-3-(2H)-thiophenone]	64	0.412	0.380	42,501	0.369	17	124	29	112	123	111 duplicate
5594	49 [877; Pyrophosphoric ac	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	0.404	0.478	11,179	0.416	18	123	18	123	11	84 original
5624	49 [877; Pyrophosphoric ac	81	Tyrosine	64	0.401	0.404	46,754	0.474	19	122	26	115	131	35 original
5602	49 [877; Pyrophosphoric ac	59	Ornithine; Arginine	64	0.388	0.293	54,605	0.378	20	121	32	109	138	102 original
5604	49 [877; Pyrophosphoric ac	61	[NA]	64	0.374	0.415	18,478	0.415	21	120	24	117	44	85 original
14050	49 [877; Pyrophosphoric ac	34	Aspartic acid	64	0.369	0.399	46,033	0.378	22	119	27	114	130	107 duplicate
5595	49 [877; Pyrophosphoric ac	52	[NA]	48	0.360	0.602	10,441	0.441	23	118	13	128	6	67 original
10943	49 [877; Pyrophosphoric ac	8	Isoleucine	55	0.347	0.270	29,485	0.340	24	117	35	106	95	135 duplicate
14968	49 [877; Pyrophosphoric ac	43	[548; Leucine (2TBS)]	60	0.329	0.472	18,811	0.421	25	116	19	122	49	81 duplicate
10268	49 [877; Pyrophosphoric ac	3	Ethanolamine	62	0.306	0.407	13,048	0.457	26	115	25	116	18	48 duplicate
12818	49 [877; Pyrophosphoric ac	23	Homoserine	64	0.306	0.545	19,640	0.448	27	114	14	127	54	60 duplicate
13835	49 [877; Pyrophosphoric ac	32	[729; N,N-Dimethyllysine methyl ester]	63	0.295	0.387	15,748	0.455	28	113	28	113	30	52 duplicate
5611	49 [877; Pyrophosphoric ac	68	[570; Hypoxanthine (2TMS)]	20	0.295	0.533	10,263	0.408	29	112	15	126	5	87 original
5641	49 [877; Pyrophosphoric ac	98	[697; Ribose-5-phosphate methoxamine (5TMS)]	48	0.284	0.470	10,489	0.407	30	111	20	121	8	88 original
13280	49 [877; Pyrophosphoric ac	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	0.279	0.495	12,575	0.449	31	110	16	125	15	58 duplicate
13726	49 [877; Pyrophosphoric ac	31	[622; Parabenic acid (2TMS)]	64	0.267	0.361	13,305	0.388	32	109	30	111	21	97 duplicate
11075	49 [877; Pyrophosphoric ac	9	Proline	63	0.242	0.166	39,670	0.342	33	108	44	97	117	134 duplicate
5651	49 [877; Pyrophosphoric ac	108	Octadecenoic acid	64	0.238	0.259	16,338	0.353	34	107	36	105	33	127 original
14365	49 [877; Pyrophosphoric ac	37	Phenylalanine	64	0.236	0.229	36,861	0.375	35	106	38	103	112	108 duplicate
5650	49 [877; Pyrophosphoric ac	107	9-(Z)-Octadecenoic acid	64	0.207	0.293	28,480	0.349	36	105	33	108	91	131 original
9991	49 [877; Pyrophosphoric ac	1	[938; Sulfuric acid (2TMS)]	36	0.206	0.206	17,136	0.472	37	104	40	101	38	37 duplicate
5636	49 [877; Pyrophosphoric ac	93	[607; Putrescine (4TMS)]	60	0.206	0.281	12,249	0.360	38	103	34	107	14	122 original
5610	49 [877; Pyrophosphoric ac	67	Citric acid	64	0.191	0.184	37,992	0.384	39	102	42	99	115	99 original
5615	49 [877; Pyrophosphoric ac	72	[919; D-Xylopyranose (4TMS)]	63	0.190	0.204	16,713	0.372	40	101	41	100	35	110 original
5633	49 [877; Pyrophosphoric ac	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	64	0.172	0.258	20,377	0.352	41	100	37	104	56	128 original
5596	49 [877; Pyrophosphoric ac	53	Glycerol-2-phosphate	64	0.156	0.305	12,929	0.340	42	98	31	110	17	136 original
5609	49 [877; Pyrophosphoric ac	66	Glyceric acid-3-phosphate	64	0.154	0.148	16,756	0.364	43	99	45	96	38	116 original
5603	49 [877; Pyrophosphoric ac	60	Glycerol-3-phosphate	64	0.154	0.123	35,566	0.361	44	97	48	93	111	120 original
5627	49 [877; Pyrophosphoric ac	84	Mannitol	62	0.153	0.094	44,234	0.378	45	96	46	95	125	105 original
10130	49 [877; Pyrophosphoric ac	4	Serine	62	0.148	0.094	30,612	0.364	46	95	49	92	97	118 duplicate
15350	49 [877; Pyrophosphoric ac	27	[NA]	64	0.108	0.218	20,480	0.421	47	94	39	102	57	82 duplicate
5642	49 [877; Pyrophosphoric ac	99	[662; Ribose-5-phosphate methoxamine (BP) (5TMS)]	41	0.102	-0.250	16,239	0.486	48	93	68	73	32	27 original
5662	49 [877; Pyrophosphoric ac	119	[931; myo-Inositol-2-phosphate (7TMS)]	64	0.098	0.172	20,729	0.432	49	92	43	98	59	73 original
10405	49 [877; Pyrophosphoric ac	4	Phosphoric acid	51	0.062	0.130	45,991	0.324	50	91	47	94	128	138 duplicate
10810	49 [877; Pyrophosphoric ac	7	Threonine	64	0.060	0.029	44,367	0.344	51	90	51	90	128	132 duplicate

14261	49 [877; Pyrophosphoric ac	38	[596; N-Acetylglutamic acid (2TMS)]	64	0.036	0.010	42,747	0.367	52	89	52	89	124	112 duplicate
5618	49 [877; Pyrophosphoric ac	75	Lysine	64	0.005	-0.027	53,787	0.354	53	88	56	85	137	128 original
5667	49 [877; Pyrophosphoric ac	124	[734; 1-Monodeoxyglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	59	-0.023	0.042	14,097	0.361	54	87	50	91	23	121 original
5673	49 [877; Pyrophosphoric ac	130	Trehalose	63	-0.026	-0.084	44,375	0.359	55	88	60	81	127	125 original
5679	49 [877; Pyrophosphoric ac	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.029	-0.005	14,693	0.365	56	85	54	87	25	115 original
5601	49 [877; Pyrophosphoric ac	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	-0.032	-0.059	30,200	0.339	57	84	59	82	96	137 original
5640	49 [877; Pyrophosphoric ac	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	-0.038	-0.020	34,496	0.406	58	83	55	86	109	89 original
5680	49 [877; Pyrophosphoric ac	137	Ergosterol	64	-0.073	-0.132	28,206	0.351	59	82	63	78	90	129 original
5670	49 [877; Pyrophosphoric ac	127	[777; Fructose-6-phosphate methoxamine (6TMS)]	39	-0.074	-0.106	18,701	0.393	60	81	62	79	48	95 original
5648	49 [877; Pyrophosphoric ac	105	[705; 2-Ketogluconic acid (5TMS)]	48	-0.074	-0.043	25,127	0.434	61	80	58	83	77	70 original
5682	49 [877; Pyrophosphoric ac	139	[700; Ergosta-5,7-dien-3-ol]	38	-0.075	0.008	11,196	0.271	62	79	53	88	12	140 original
5634	49 [877; Pyrophosphoric ac	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	-0.095	-0.027	27,558	0.366	63	78	57	84	88	113 original
5684	49 [877; Pyrophosphoric ac	141	[Lanosta-8,24-dien-3-beta-ol]	61	-0.108	-0.190	14,538	0.363	64	77	66	75	24	119 original
5671	49 [877; Pyrophosphoric ac	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	-0.115	-0.171	22,584	0.390	65	76	65	76	67	96 original
5614	49 [877; Pyrophosphoric ac	71	[731; Erythrose (3TMS)]	64	-0.125	-0.233	26,698	0.394	66	75	67	74	82	94 original
5661	49 [877; Pyrophosphoric ac	118	[928; Glucopyranose-6-phosphate (6TMS)]	58	-0.131	-0.285	18,965	0.378	67	74	71	70	51	104 original
5654	49 [877; Pyrophosphoric ac	111	[583; Erythritol (4TMS)]	42	-0.182	-0.259	11,723	0.359	68	73	69	72	13	123 original
5637	49 [877; Pyrophosphoric ac	94	Hexadecanoic acid	64	-0.188	-0.559	37,209	0.474	69	72	97	44	113	36 original
5644	49 [877; Pyrophosphoric ac	101	[832; Dopamine (4TMS)]	64	-0.202	-0.159	23,715	0.359	70	71	64	77	74	124 original
5605	49 [877; Pyrophosphoric ac	64	[789; Tyramine (3TMS)]	63	-0.208	-0.302	18,312	0.350	71	70	73	68	42	130 original
5635	49 [877; Pyrophosphoric ac	92	[680; Glycerol-2-phosphate (4TMS)]	54	-0.210	-0.460	21,957	0.402	72	69	83	58	62	92 original
11846	49 [877; Pyrophosphoric ac	15	Alanine	64	-0.212	-0.360	33,491	0.423	73	68	75	66	108	79 duplicate
5652	49 [877; Pyrophosphoric ac	109	Octadecanoic acid	64	-0.227	-0.660	38,535	0.504	74	67	121	20	116	13 original
5623	49 [877; Pyrophosphoric ac	80	[772; D-Glucose (5TMS)]	62	-0.240	-0.440	45,144	0.377	75	66	81	60	128	106 original
5646	49 [877; Pyrophosphoric ac	103	[648; Ethylamine (2TMS)]	63	-0.269	-0.279	27,676	0.397	76	65	70	71	88	93 original
5681	49 [877; Pyrophosphoric ac	138	[674; Ergosterol (1TMS)]	46	-0.273	-0.395	13,285	0.420	77	64	79	62	20	83 original
5678	49 [877; Pyrophosphoric ac	135	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	-0.282	-0.452	26,915	0.388	78	63	82	59	84	98 original
5683	49 [877; Pyrophosphoric ac	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	49	-0.284	-0.366	13,080	0.364	79	62	78	63	19	117 original
5597	49 [877; Pyrophosphoric ac	54	[NA]	55	-0.285	-0.438	18,339	0.444	80	61	80	61	43	63 original
5600	49 [877; Pyrophosphoric ac	116	[757; 2-Desoxy-pentose-3-ylose dimethoxamine (2TMS)]	55	-0.280	-0.541	28,889	0.442	81	60	93	48	92	64 original
5676	49 [877; Pyrophosphoric ac	133	[855; Squalene]	64	-0.291	-0.294	21,644	0.374	82	59	72	69	60	109 original
5630	49 [877; Pyrophosphoric ac	87	[945; beta-D-Glucopyranose (5TMS)]	62	-0.302	-0.522	50,592	0.430	83	58	89	52	136	74 original
5622	49 [877; Pyrophosphoric ac	79	Glucose	64	-0.305	-0.522	50,057	0.463	84	57	90	51	135	41 original
5659	49 [877; Pyrophosphoric ac	116	[882; Pseudouridine (5TMS)]	30	-0.315	-0.367	17,000	0.382	85	56	76	65	37	101 original
5628	49 [877; Pyrophosphoric ac	83	Sorbitol	58	-0.319	-0.105	34,761	0.343	86	55	61	80	110	133 original
5628	49 [877; Pyrophosphoric ac	85	[529; Methylcitric acid (4TMS)]	48	-0.332	-0.843	17,435	0.422	87	54	118	23	39	80 original
5655	49 [877; Pyrophosphoric ac	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	-0.334	-0.476	12,692	0.383	88	53	85	56	16	100 original
5631	49 [877; Pyrophosphoric ac	88	Gluconic acid	64	-0.346	-0.510	27,642	0.504	89	52	86	55	87	12 original
5663	49 [877; Pyrophosphoric ac	120	[945; Uridine (3TMS)]	54	-0.352	-0.368	26,727	0.444	90	51	77	64	83	62 original
5639	49 [877; Pyrophosphoric ac	96	myo-Inositol	49	-0.364	-0.316	13,427	0.300	91	50	74	67	22	139 original
5672	49 [877; Pyrophosphoric ac	129	[840; Maltose methoxamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	-0.373	-0.538	25,200	0.478	92	49	92	49	78	31 original
5645	49 [877; Pyrophosphoric ac	102	[904; Galactose methoxamine (5TMS)]	64	-0.374	-0.463	17,908	0.403	93	48	84	57	40	91 original
11465	49 [877; Pyrophosphoric ac	12	Glyceric acid	63	-0.375	-0.561	15,758	0.441	94	47	98	43	31	68 duplicate
5593	49 [877; Pyrophosphoric ac	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	-0.378	-0.521	14,873	0.465	95	46	88	53	27	40 original
10876	49 [877; Pyrophosphoric ac	6	Glycerol	64	-0.392	-0.563	56,412	0.430	96	45	99	42	140	75 duplicate
5677	49 [877; Pyrophosphoric ac	134	Isomaltose	64	-0.393	-0.595	41,322	0.480	97	44	109	33	120	30 original

15256	49 [877; Pyrophosphoric ac 46	Arabinose	64 -0.394	-0.590	33.395	0.466	98	43	105	36	106	39 duplicate
5608	49 [877; Pyrophosphoric ac 65	[646; 3-Deoxyglucitol (5TMS)]	63 -0.395	-0.608	25.972	0.455	99	42	110	31	80	53 original
12095	49 [877; Pyrophosphoric ac 17	[700; 2-methyl-1,2-propanediol (2TMS)]	64 -0.404	-0.525	33.331	0.426	100	41	91	50	105	78 duplicate
5599	49 [877; Pyrophosphoric ac 56	[829; Oroic acid (3TMS)]	64 -0.410	-0.593	23.224	0.458	101	40	107	34	71	45 original
14771	49 [877; Pyrophosphoric ac 41	[639; Proline (2TMS)]	64 -0.421	-0.589	29.177	0.445	102	39	103	38	93	61 duplicate
13505	49 [877; Pyrophosphoric ac 29	Erythritol	64 -0.424	-0.553	19.453	0.499	103	38	98	45	52	19 duplicate
5675	49 [877; Pyrophosphoric ac 132	[895; Isomaltose methoxyamine (8TMS)]	42 -0.433	-0.595	18.553	0.463	104	37	109	32	45	42 original
5643	49 [877; Pyrophosphoric ac 100	[857; Mannitol (6TMS)]	64 -0.436	-0.516	23.965	0.426	105	36	87	54	75	77 original
11593	49 [877; Pyrophosphoric ac 13	Uracil	64 -0.437	-0.569	32.239	0.494	106	35	100	41	102	22 duplicate
14570	49 [877; Pyrophosphoric ac 39	[829; 1-Phenylethanol (1TMS)]	63 -0.437	-0.592	32.372	0.477	107	34	108	35	103	33 duplicate
5647	49 [877; Pyrophosphoric ac 104	[795; Erythritol (4TMS)]	63 -0.437	-0.646	22.396	0.455	108	34	119	22	66	49 original
5605	49 [877; Pyrophosphoric ac 62	[812; D-Xylofuranose (4TMS)]	64 -0.438	-0.587	29.394	0.459	109	32	102	39	94	44 original
12935	49 [877; Pyrophosphoric ac 24	[725; 2-Ketocacetic acid (2TMS)]	64 -0.444	-0.590	47.470	0.483	110	31	104	37	132	29 duplicate
5629	49 [877; Pyrophosphoric ac 86	[793; D-Galactono-1,4-lactone (4TMS)]	61 -0.445	-0.638	37.685	0.490	111	30	116	25	114	25 original
5666	49 [877; Pyrophosphoric ac 123	[945; Galactofuranose-6-phosphate (7TMS)]	64 -0.447	-0.634	26.254	0.428	112	29	115	26	81	76 original
11971	49 [877; Pyrophosphoric ac 16	[844; 2-Methyl-1,3-butanediol (2TMS)]	64 -0.448	-0.575	33.470	0.506	113	28	101	40	107	11 duplicate
11338	49 [877; Pyrophosphoric ac 11	Succinic acid	64 -0.450	-0.615	23.055	0.449	114	27	111	30	69	59 duplicate
5668	49 [877; Pyrophosphoric ac 125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64 -0.463	-0.642	47.732	0.437	115	26	117	24	133	69 original
14468	49 [877; Pyrophosphoric ac 38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64 -0.477	-0.624	23.248	0.475	116	24	112	29	72	34 duplicate
12340	49 [877; Pyrophosphoric ac 19	Alanine (BP) (3TMS)	64 -0.477	-0.677	27.906	0.441	117	25	126	15	89	66 duplicate
5617	49 [877; Pyrophosphoric ac 74	[912; Tetradecanoic acid (1TMS)]	64 -0.480	-0.742	23.649	0.503	118	23	137	4	73	15 original
12700	49 [877; Pyrophosphoric ac 22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52 -0.481	-0.547	15.497	0.453	119	22	94	47	29	54 duplicate
11720	49 [877; Pyrophosphoric ac 14	Fumaric acid	64 -0.492	-0.631	16.639	0.451	120	21	114	27	34	55 duplicate
12581	49 [877; Pyrophosphoric ac 21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64 -0.495	-0.628	31.937	0.434	121	19	113	28	100	71 duplicate
12218	49 [877; Pyrophosphoric ac 18	[590; 1-Acetyl-2-thiohydantoin]	64 -0.495	-0.664	23.061	0.458	122	20	122	19	70	46 duplicate
5613	49 [877; Pyrophosphoric ac 70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57 -0.503	-0.551	32.781	0.451	123	18	95	46	104	57 original
13166	49 [877; Pyrophosphoric ac 26	Citramalic acid	64 -0.512	-0.680	31.219	0.498	124	17	127	14	98	20 duplicate
5636	49 [877; Pyrophosphoric ac 113	Galactose-6-phosphate	62 -0.519	-0.702	20.664	0.457	125	16	131	10	58	47 original
5657	49 [877; Pyrophosphoric ac 114	Fructose-6-phosphate	53 -0.522	-0.686	18.697	0.460	126	15	129	12	47	43 original
13393	49 [877; Pyrophosphoric ac 28	Malic acid	64 -0.538	-0.676	24.669	0.493	127	14	125	16	76	24 duplicate
5669	49 [877; Pyrophosphoric ac 126	[559; Erythritol (4TMS)]	45 -0.539	-0.684	19.816	0.546	128	13	128	13	53	1 original
5621	49 [877; Pyrophosphoric ac 78	Mannose	62 -0.556	-0.674	22.329	0.515	129	12	123	18	64	7 original
14156	49 [877; Pyrophosphoric ac 35	Pyroglutamic acid	64 -0.571	-0.674	56.154	0.488	130	11	124	17	139	26 duplicate
5665	49 [877; Pyrophosphoric ac 122	[644; Erythritol (4TMS)]	52 -0.573	-0.657	18.922	0.520	131	10	120	21	50	6 original
5658	49 [877; Pyrophosphoric ac 115	Glucose-6-phosphate	62 -0.575	-0.694	40.400	0.455	132	9	130	11	119	51 original
5616	49 [877; Pyrophosphoric ac 73	[708; Glucose methoxyamine (5TMS)]	57 -0.580	-0.727	21.952	0.512	133	8	134	7	61	9 original
5653	49 [877; Pyrophosphoric ac 110	[715; Erythritol (4TMS)]	54 -0.586	-0.717	22.931	0.503	134	7	133	8	68	14 original
5660	49 [877; Pyrophosphoric ac 117	[724; Glycerol (3TMS)]	56 -0.587	-0.705	22.324	0.470	135	6	132	9	63	38 original
14671	49 [877; Pyrophosphoric ac 40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64 -0.597	-0.741	49.030	0.499	136	5	136	5	134	18 duplicate
15065	49 [877; Pyrophosphoric ac 44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	50 -0.603	-0.758	25.594	0.523	137	4	140	1	79	4 duplicate
5664	49 [877; Pyrophosphoric ac 121	[657; Erythritol (4TMS)]	55 -0.616	-0.747	18.017	0.523	138	3	138	3	41	5 original
5649	49 [877; Pyrophosphoric ac 106	[733; Threitol (4TMS)]	62 -0.633	-0.755	26.945	0.528	139	2	139	2	85	3 original
5619	49 [877; Pyrophosphoric ac 76	Fructose	64 -0.663	-0.732	41.949	0.507	140	1	135	6	122	10 original
5699	50 [746; Ribonic acid-1,4-le	55 [646; 3-Deoxyglucitol (5TMS)]	60 0.819	0.852	16.399	0.627	1	140	7	134	53	8 original
5691	50 [746; Ribonic acid-1,4-le	57 [757; 2-Desoxy-pentose-3-ylose dimethoxyamine (2TMS)]	55 0.815	0.929	21.073	0.597	2	139	13	128	76	26 original
5763	50 [746; Ribonic acid-1,4-le	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	58 0.811	0.961	17.257	0.613	3	138	3	138	57	20 original
15257	50 [746; Ribonic acid-1,4-le	46 Arabinose	61 0.808	0.931	27.190	0.624	4	137	11	130	93	12 duplicate
5720	50 [746; Ribonic acid-1,4-le	86 [793; D-Galactono-1,4-lactone (4TMS)]	58 0.806	0.901	31.207	0.617	5	136	16	125	104	15 original
11594	50 [746; Ribonic acid-1,4-le	13 Uracil	61 0.797	0.970	28.517	0.661	6	134	1	140	97	2 duplicate

12836	50 [746; Ribonic acid-1,4-le 24	1725; 2-Ketooctanoic acid (2TMS)]	0.658	7	135	2	139	130	33uplicate
11972	50 [746; Ribonic acid-1,4-le 16	[644; 2-Methyl-1,3-butanediol (2TMS)]	0.689	8	133	4	137	103	1uplicate
5768	50 [746; Ribonic acid-1,4-le 134	Isomaltose	0.959	30,944	0.689	8	133	103	14 original
5690	50 [746; Ribonic acid-1,4-le 56	[829; Oroic acid (3TMS)]	0.954	37,125	0.623	9	132	5	138 116
14571	50 [746; Ribonic acid-1,4-le 39	[829; 1-Phenylethanol (1TMS)]	0.930	14,703	0.624	10	131	12	129 40
13508	50 [746; Ribonic acid-1,4-le 29	Erythritol	0.953	26,750	0.626	11	130	8	135 91
5722	50 [746; Ribonic acid-1,4-le 88	Gluconic acid	0.941	16,038	0.649	12	129	8	133 50
14069	50 [746; Ribonic acid-1,4-le 17	[700; 2-methyl-1,2-propanediol (2TMS)]	0.895	23,016	0.648	13	128	17	124 83
14489	50 [746; Ribonic acid-1,4-le 38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	0.910	30,570	0.614	14	127	15	126 102
5696	50 [746; Ribonic acid-1,4-le 62	[812; D-Xylofuranose (4TMS)]	0.938	19,610	0.634	15	126	9	132 69
5733	50 [746; Ribonic acid-1,4-le 99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	0.880	27,426	0.585	16	125	20	121 95
5688	50 [746; Ribonic acid-1,4-le 54	[NA]	0.932	6,886	0.638	17	124	10	131 6
11337	50 [746; Ribonic acid-1,4-le 11	Succinic acid	0.871	9,458	0.560	18	123	21	120 19
11721	50 [746; Ribonic acid-1,4-le 14	Fumaric acid	0.861	20,087	0.570	19	122	22	119 70
5726	50 [746; Ribonic acid-1,4-le 92	[680; Glycerol-2-phosphate (4TMS)]	0.916	10,811	0.606	20	121	14	127 23
5704	50 [746; Ribonic acid-1,4-le 70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	0.708	15,110	0.506	21	120	42	99 45
11488	50 [746; Ribonic acid-1,4-le 105	[705; 2-Ketogluconic acid (5TMS)]	0.549	31,298	0.445	22	119	59	82 105
5737	50 [746; Ribonic acid-1,4-le 103	[648; Ethylamine (2TMS)]	0.841	8,730	0.589	23	118	25	118 13
12701	50 [746; Ribonic acid-1,4-le 22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	0.859	18,931	0.567	24	117	23	118 64
5739	50 [746; Ribonic acid-1,4-le 78	Mannose	0.816	22,899	0.567	25	116	27	114 82
13394	50 [746; Ribonic acid-1,4-le 28	Malic acid	0.866	6,951	0.583	26	115	19	122 8
5731	50 [746; Ribonic acid-1,4-le 97	[756; beta-D-Methylglucopyranoside (4TMS)]	0.779	14,052	0.528	27	114	33	108 36
5740	50 [746; Ribonic acid-1,4-le 108	[733; Threitol (4TMS)]	0.888	22,017	0.612	28	113	18	123 78
5707	50 [746; Ribonic acid-1,4-le 73	[708; Glucose methoxyamine (5TMS)]	0.789	29,926	0.516	29	112	31	110 88
14672	50 [746; Ribonic acid-1,4-le 40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	0.817	20,385	0.596	30	111	26	115 73
9992	50 [746; Ribonic acid-1,4-le 1	[938; Sulfuric acid (2TMS)]	0.698	14,978	0.476	31	110	44	97 44
5710	50 [746; Ribonic acid-1,4-le 76	Fructose	0.810	48,329	0.559	32	109	28	113 135
12582	50 [746; Ribonic acid-1,4-le 21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	0.673	10,184	0.587	33	108	48	93 22
5759	50 [746; Ribonic acid-1,4-le 125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	0.806	38,537	0.571	34	107	29	112 119
5735	50 [746; Ribonic acid-1,4-le 101	[832; Dopamine (4TMS)]	0.752	30,094	0.513	35	106	36	105 100
13167	50 [746; Ribonic acid-1,4-le 26	Citramalic acid	0.713	45,400	0.506	36	105	41	100 129
5762	50 [746; Ribonic acid-1,4-le 128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	0.724	20,177	0.498	37	104	39	102 71
5754	50 [746; Ribonic acid-1,4-le 120	[945; Uridine (3TMS)]	0.750	30,058	0.495	38	103	37	104 89
5749	50 [746; Ribonic acid-1,4-le 115	Glucose-6-phosphate	0.783	16,133	0.574	39	102	32	109 51
5756	50 [746; Ribonic acid-1,4-le 122	[644; Erythritol (4TMS)]	0.388	23,676	0.610	40	101	68	73 84
5721	50 [746; Ribonic acid-1,4-le 35	Pyrogutamic acid	0.741	37,958	0.551	41	100	38	103 118
14157	50 [746; Ribonic acid-1,4-le 91	[768; beta-D-Methylglucopyranoside (4TMS)]	0.806	8,311	0.562	42	99	30	111 11
5725	50 [746; Ribonic acid-1,4-le 91	[768; beta-D-Methylglucopyranoside (4TMS)]	0.889	48,288	0.463	43	98	47	94 134
5755	50 [746; Ribonic acid-1,4-le 121	[657; Erythritol (4TMS)]	0.769	55,150	0.568	44	97	35	106 139
5744	50 [746; Ribonic acid-1,4-le 110	[715; Erythritol (4TMS)]	0.672	24,321	0.454	45	96	49	92 86
5719	50 [746; Ribonic acid-1,4-le 85	[528; Methylcitric acid (4TMS)]	0.686	6,898	0.548	46	95	45	96 7
5751	50 [746; Ribonic acid-1,4-le 117	[724; Glycerol (3TMS)]	0.771	13,100	0.615	47	94	34	107 33
5734	50 [746; Ribonic acid-1,4-le 100	[857; Mannitol (6TMS)]	0.703	15,912	0.447	48	93	43	98 48
5738	50 [746; Ribonic acid-1,4-le 102	[904; Galactose methoxyamine (5TMS)]	0.723	14,413	0.552	49	92	40	101 38
10677	50 [746; Ribonic acid-1,4-le 6	Glycerol	0.693	21,536	0.547	50	91	46	95 77
5748	50 [746; Ribonic acid-1,4-le 112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	0.581	14,411	0.522	51	90	55	86 37
15066	50 [746; Ribonic acid-1,4-le 44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	0.597	55,616	0.481	52	89	52	89 140
5766	50 [746; Ribonic acid-1,4-le 132	[895; Isomaltose methoxyamine (8TMS)]	0.615	5,104	0.500	53	88	51	90 1
5708	50 [746; Ribonic acid-1,4-le 74	[912; Tetradecanoic acid (1TMS)]	0.666	17,374	0.583	54	87	50	91 58
12219	50 [746; Ribonic acid-1,4-le 18	[590; 1-Acetyl-2-thiohydantoin]	0.855	8,837	0.591	55	86	24	117 14
			0.529	16,608	0.533	56	85	60	81 54
			0.457	20,397	0.422	57	84	64	77 74

5760	50 [746; Ribonic acid-1,4-le	126	[559; Erythritol (4TMS)]	45	0.285	0.517	11,187	0.593	58	83	62	79	26	30	original
5761	50 [746; Ribonic acid-1,4-le	127	[777; Fructose-6-phosphate methoxyamine (5TMS)]	39	0.279	0.595	11,234	0.616	59	82	53	88	27	16	original
5769	50 [746; Ribonic acid-1,4-le	135	[902; Melibiose (8TMS); alpha-D-GalH(1,6)-D-Glc (8TMS)]	61	0.273	0.509	25,764	0.435	60	81	63	78	88	107	original
5714	50 [746; Ribonic acid-1,4-le	80	[772; D-Glucose (5TMS)]	59	0.265	0.562	43,735	0.424	61	80	58	83	124	116	original
12341	50 [746; Ribonic acid-1,4-le	19	Alanine (BP) (3TMS)	61	0.247	0.520	24,729	0.467	62	79	61	80	87	89	duplicate
5750	50 [746; Ribonic acid-1,4-le	116	[882; Pseudouridine (5TMS)]	29	0.246	0.414	11,318	0.257	63	78	66	75	29	140	original
5738	50 [746; Ribonic acid-1,4-le	104	[795; Erythritol (4TMS)]	60	0.235	0.420	17,933	0.501	64	77	65	76	59	73	original
15351	50 [746; Ribonic acid-1,4-le	47	[NA]	61	0.232	0.314	19,340	0.470	65	76	71	70	67	88	duplicate
5747	50 [746; Ribonic acid-1,4-le	113	Galactose-6-phosphate	59	0.225	0.592	44,033	0.490	66	75	54	87	35	81	original
5718	50 [746; Ribonic acid-1,4-le	84	Mannitol	59	0.222	0.575	44,269	0.509	67	74	56	85	127	66	original
14772	50 [746; Ribonic acid-1,4-le	41	[639; Proline (2TMS)]	61	0.212	0.390	27,010	0.424	68	73	67	74	92	117	duplicate
6687	50 [746; Ribonic acid-1,4-le	53	Glycerol-2-phosphate	61	0.191	0.179	10,065	0.355	69	72	78	83	21	135	original
5748	50 [746; Ribonic acid-1,4-le	114	Fructose-6-phosphate	52	0.173	0.570	11,273	0.509	70	71	57	84	28	67	original
5727	50 [746; Ribonic acid-1,4-le	93	[607; Putrescine (4TMS)]	57	0.168	0.353	8,705	0.363	71	70	70	71	12	132	original
5730	50 [746; Ribonic acid-1,4-le	96	myo-Inositol	46	0.136	0.164	5,581	0.292	72	69	80	61	3	139	original
5774	50 [746; Ribonic acid-1,4-le	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	46	0.125	0.266	5,167	0.429	73	68	74	87	2	113	original
5757	50 [746; Ribonic acid-1,4-le	123	[945; Galactofuranose-6-phosphate (7TMS)]	61	0.120	0.311	24,129	0.475	74	67	72	69	85	86	original
5724	50 [746; Ribonic acid-1,4-le	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	61	0.097	0.149	19,203	0.362	75	66	81	60	66	133	original
5767	50 [746; Ribonic acid-1,4-le	133	[855; Squalene]	61	0.096	0.014	18,999	0.433	76	65	84	57	65	108	original
5717	50 [746; Ribonic acid-1,4-le	83	Sorbitol	55	0.067	-0.368	34,713	0.377	77	64	94	47	110	129	original
5743	50 [746; Ribonic acid-1,4-le	109	Octadecanoic acid	61	0.058	0.297	34,857	0.431	78	63	73	68	112	111	original
5775	50 [746; Ribonic acid-1,4-le	141	Lanosta-8,24-dien-3-beta-ol	58	0.055	0.189	8,992	0.428	79	62	77	64	16	114	original
5745	50 [746; Ribonic acid-1,4-le	111	[583; Erythritol (4TMS)]	42	0.038	0.198	7,093	0.430	80	61	76	65	9	112	original
5728	50 [746; Ribonic acid-1,4-le	94	Hexadecanoic acid	61	0.009	0.236	34,848	0.455	81	60	75	66	111	94	original
5713	50 [746; Ribonic acid-1,4-le	79	Glucose	61	0.008	0.360	48,900	0.504	82	59	69	72	136	71	original
5706	50 [746; Ribonic acid-1,4-le	72	[919; D-Xylopyranose (4TMS)]	60	0.002	-0.035	15,618	0.343	83	58	87	54	47	137	original
11847	50 [746; Ribonic acid-1,4-le	15	Alanine	61	-0.015	0.135	32,347	0.555	84	57	82	59	108	49	duplicate
5698	50 [746; Ribonic acid-1,4-le	64	[769; Tyramine (3TMS)]	57	-0.020	0.089	16,249	0.388	85	56	83	58	52	127	original
5752	50 [746; Ribonic acid-1,4-le	118	[928; Glucopyranose-6-phosphate (5TMS)]	57	-0.024	0.167	14,846	0.410	86	55	79	62	42	121	original
5697	50 [746; Ribonic acid-1,4-le	63	Glutamine	49	-0.032	-0.610	18,880	0.625	87	54	107	34	63	10	original
5773	50 [746; Ribonic acid-1,4-le	139	[700; Ergosta-5,7-dien-3-ol]	35	-0.035	-0.087	6,607	0.357	88	53	88	53	4	134	original
5771	50 [746; Ribonic acid-1,4-le	137	Ergosterol	61	-0.042	-0.127	26,726	0.370	89	52	90	51	90	130	original
5741	50 [746; Ribonic acid-1,4-le	107	9-(Z)-Octadecenoic acid	61	-0.049	-0.116	27,996	0.386	90	51	89	52	96	128	original
5753	50 [746; Ribonic acid-1,4-le	119	[931; myo-Inositol-2-phosphate (7TMS)]	61	-0.051	0.007	19,550	0.397	91	50	85	56	68	125	original
5772	50 [746; Ribonic acid-1,4-le	138	[674; Ergosterol (1TMS)]	43	-0.083	0.006	6,777	0.438	92	49	86	55	5	104	original
5758	50 [746; Ribonic acid-1,4-le	124	[734; 1-Monooctylglycerol (2TMS); 1-Monohexadecylglycerol (1TMS)]	56	-0.134	-0.234	9,235	0.401	93	48	91	50	17	123	original
5688	50 [746; Ribonic acid-1,4-le	52	[NA]	43	-0.163	-0.493	14,758	0.564	94	47	99	42	41	43	original
5764	50 [746; Ribonic acid-1,4-le	130	Trehalose	61	-0.185	-0.282	44,011	0.384	95	46	92	49	125	131	original
10406	50 [746; Ribonic acid-1,4-le	4	Phosphoric acid	48	-0.216	-0.494	46,393	0.329	96	45	100	41	131	138	duplicate
5705	50 [746; Ribonic acid-1,4-le	71	[731; Erythrose (3TMS)]	61	-0.245	-0.342	25,920	0.401	97	44	93	48	89	122	original
14969	50 [746; Ribonic acid-1,4-le	43	[548; Leucine (2TBS)]	57	-0.264	-0.451	20,513	0.416	98	43	98	43	75	120	duplicate
5742	50 [746; Ribonic acid-1,4-le	108	Octadecenoic acid	61	-0.264	-0.419	15,565	0.397	99	42	95	46	46	124	original
5770	50 [746; Ribonic acid-1,4-le	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.279	-0.421	8,080	0.433	100	41	98	45	10	110	original
13052	50 [746; Ribonic acid-1,4-le	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.303	-0.886	18,236	0.624	101	40	134	7	60	13	duplicate
5695	50 [746; Ribonic acid-1,4-le	61	[NA]	61	-0.331	-0.435	18,246	0.421	102	39	97	44	61	119	original
5692	50 [746; Ribonic acid-1,4-le	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	61	-0.350	-0.527	30,118	0.433	103	38	102	39	101	109	original
14262	50 [746; Ribonic acid-1,4-le	36	[596; N-Acetylglutamic acid (2TMS)]	61	-0.363	-0.607	42,850	0.450	104	37	108	35	121	99	duplicate
5732	50 [746; Ribonic acid-1,4-le	98	[597; Ribose-5-phosphate methoxyamine (5TMS)]	45	-0.364	-0.753	12,128	0.556	105	36	119	22	31	48	original

15538	50 [746; Ribonic acid-1,4-di	49	[877; Pyrophosphoric acid (4TMS)]	61	-0.378	-0.521	14,873	0.465	106	35	101	40	43	90	duplicate
5708	50 [746; Ribonic acid-1,4-di	75	Lysine	61	-0.384	-0.814	53,685	0.453	107	34	108	33	137	98	original
13281	50 [746; Ribonic acid-1,4-di	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	50	-0.401	-0.844	18,635	0.537	108	33	129	12	62	55	duplicate
12819	50 [746; Ribonic acid-1,4-di	23	Homoserine	61	-0.407	-0.839	22,808	0.589	109	32	128	13	81	32	duplicate
5723	50 [746; Ribonic acid-1,4-di	89	[775; Dopamine (4TMS)]	32	-0.411	-0.725	17,142	0.425	110	31	116	25	56	115	original
5765	50 [746; Ribonic acid-1,4-di	131	[626; 5-Methylthioadenosine (3TMS)]	52	-0.416	-0.563	9,285	0.496	111	30	103	38	18	76	original
5729	50 [746; Ribonic acid-1,4-di	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	47	-0.475	-0.604	10,908	0.437	112	29	105	38	24	106	original
10811	50 [746; Ribonic acid-1,4-di	7	Threonine	61	-0.484	-0.650	44,334	0.438	113	28	111	30	128	105	duplicate
5700	50 [746; Ribonic acid-1,4-di	66	Glyceral acid-3-phosphate	61	-0.501	-0.712	16,001	0.493	114	27	115	26	49	80	original
15444	50 [746; Ribonic acid-1,4-di	48	Asparagine	61	-0.508	-0.797	22,660	0.594	115	28	128	15	80	29	duplicate
5701	50 [746; Ribonic acid-1,4-di	67	Citric acid	61	-0.510	-0.640	37,862	0.391	116	25	109	32	117	126	original
15162	50 [746; Ribonic acid-1,4-di	45	Homocysteine	58	-0.515	-0.846	9,959	0.440	117	24	110	31	20	103	duplicate
5694	50 [746; Ribonic acid-1,4-di	60	Glycerol-3-phosphate	61	-0.519	-0.658	35,654	0.455	118	23	112	29	114	95	original
13727	50 [746; Ribonic acid-1,4-di	31	[622; Parabanic acid (2TMS)]	61	-0.523	-0.763	13,716	0.505	119	22	120	21	34	70	duplicate
10131	50 [746; Ribonic acid-1,4-di	2	Serine	59	-0.527	-0.698	32,127	0.454	120	21	113	28	107	98	duplicate
5702	50 [746; Ribonic acid-1,4-di	68	[570; Hypoxanthine (2TMS)]	19	-0.544	-0.902	8,868	0.483	121	20	137	4	15	83	original
12462	50 [746; Ribonic acid-1,4-di	20	[619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	28	-0.556	-0.790	11,318	0.523	122	19	125	16	30	59	duplicate
10944	50 [746; Ribonic acid-1,4-di	8	Isoleucine	52	-0.557	-0.602	31,632	0.355	123	18	104	37	106	136	duplicate
14366	50 [746; Ribonic acid-1,4-di	37	Phenylalanine	61	-0.576	-0.766	36,968	0.474	124	17	122	19	115	87	duplicate
14051	50 [746; Ribonic acid-1,4-di	34	Aspartic acid	61	-0.584	-0.689	47,024	0.484	125	16	114	27	132	82	duplicate
11076	50 [746; Ribonic acid-1,4-di	5	Proline	60	-0.598	-0.737	41,340	0.449	126	15	118	23	120	100	duplicate
5689	50 [746; Ribonic acid-1,4-di	55	[812; 4-Aminobutyric acid (2TBS)]	40	-0.600	-0.735	12,146	0.460	127	14	117	24	32	92	original
13944	50 [746; Ribonic acid-1,4-di	33	Methionine	61	-0.628	-0.763	22,649	0.502	128	13	121	20	79	72	duplicate
10269	50 [746; Ribonic acid-1,4-di	3	Ethanolamine	59	-0.662	-0.822	14,685	0.495	129	12	127	14	39	77	duplicate
5685	50 [746; Ribonic acid-1,4-di	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	41	-0.676	-0.867	11,016	0.494	130	11	133	8	25	79	original
5693	50 [746; Ribonic acid-1,4-di	59	Ornithine; Arginine	61	-0.679	-0.777	54,881	0.514	131	10	124	17	138	64	original
13617	50 [746; Ribonic acid-1,4-di	30	[815; Ethyl-3(2H)-thiophenone]	61	-0.685	-0.777	44,026	0.457	132	9	123	18	128	93	duplicate
13836	50 [746; Ribonic acid-1,4-di	32	[729; N,N-Dimethyllysine methyl ester]	60	-0.689	-0.899	20,311	0.614	133	8	136	5	72	19	duplicate
5703	50 [746; Ribonic acid-1,4-di	69	Arginine	57	-0.702	-0.934	35,230	0.610	134	7	140	1	113	23	original
11207	50 [746; Ribonic acid-1,4-di	10	Glycine	61	-0.706	-0.931	33,200	0.604	135	6	139	2	109	25	duplicate
10542	50 [746; Ribonic acid-1,4-di	5	Leucine	42	-0.721	-0.867	16,759	0.521	136	5	132	9	55	61	duplicate
5711	50 [746; Ribonic acid-1,4-di	77	[826; beta-[[[5-methyl-2-thienyl)methyl]amino- benzeneacetic acid methyl ester]	59	-0.722	-0.855	43,570	0.530	137	4	130	11	123	57	original
5716	50 [746; Ribonic acid-1,4-di	82	Lysine	36	-0.743	-0.928	27,214	0.542	138	3	138	3	94	54	original
5715	50 [746; Ribonic acid-1,4-di	81	Tyrosine	61	-0.764	-0.894	47,995	0.596	139	2	135	6	133	28	original
14871	50 [746; Ribonic acid-1,4-di	42	Glutamic acid	57	-0.768	-0.865	43,218	0.516	140	1	131	10	122	62	duplicate
5792	51 [499; 2-Ethyl-3-hydroxy-	68	[570; Hypoxanthine (2TMS)]	16	0.817	0.876	2,751	0.570	1	140	3	138	1	20	original
11208	51 [499; 2-Ethyl-3-hydroxy-	10	Glycine	44	0.751	0.861	31,774	0.552	2	138	7	134	109	22	duplicate
15445	51 [499; 2-Ethyl-3-hydroxy-	48	Asparagine	44	0.751	0.844	21,331	0.580	3	139	9	132	76	14	duplicate
5805	51 [499; 2-Ethyl-3-hydroxy-	81	Tyrosine	44	0.748	0.829	45,629	0.596	4	137	11	130	136	10	original
14872	51 [499; 2-Ethyl-3-hydroxy-	42	Glutamic acid	44	0.748	0.859	42,264	0.621	5	136	8	133	129	4	duplicate
13618	51 [499; 2-Ethyl-3-hydroxy-	30	[815; Ethyl-3(2H)-thiophenone]	44	0.732	0.832	42,524	0.604	6	135	10	131	130	8	duplicate
10270	51 [499; 2-Ethyl-3-hydroxy-	3	Ethanolamine	43	0.728	0.792	13,054	0.547	7	134	18	123	28	27	duplicate
5801	51 [499; 2-Ethyl-3-hydroxy-	77	[826; beta-[[[5-methyl-2-thienyl)methyl]amino- benzeneacetic acid methyl ester]	43	0.717	0.887	41,999	0.649	8	133	1	140	128	1	original
10543	51 [499; 2-Ethyl-3-hydroxy-	5	Leucine	38	0.684	0.818	12,795	0.585	9	132	13	128	25	13	duplicate
5793	51 [499; 2-Ethyl-3-hydroxy-	69	Arginine	43	0.674	0.883	33,680	0.594	10	131	2	139	114	11	original
13945	51 [499; 2-Ethyl-3-hydroxy-	33	Methionine	44	0.658	0.802	22,342	0.604	11	130	15	126	80	9	duplicate
5860	51 [499; 2-Ethyl-3-hydroxy-	138	[748; D-Sedoheptulose-7-phosphate (7TMS)]	10	0.644	0.725	12,347	0.271	12	129	21	120	22	137	original
5806	51 [499; 2-Ethyl-3-hydroxy-	82	Lysine	32	0.641	0.871	25,249	0.573	13	128	4	137	89	18	original



5785	51 [499; 2-Ethyl-3-hydroxy- 61 [NA]	44	0.628	0.864	18,725	0.516	14	127	28	113	59	43 original
5783	51 [499; 2-Ethyl-3-hydroxy- 59 Ornithine; Arginine	44	0.600	0.868	51,028	0.577	15	125	5	136	140	15 original
14367	51 [499; 2-Ethyl-3-hydroxy- 37 Phenylalanine	44	0.600	0.788	35,101	0.572	16	126	17	124	117	19 duplicate
13053	51 [499; 2-Ethyl-3-hydroxy- 25 [709; 2,5-Diaminovalerolactam (2TMS)]	29	0.586	0.815	16,047	0.494	17	124	14	127	42	59 duplicate
5779	51 [499; 2-Ethyl-3-hydroxy- 55 [612; 4-Aminobutyric acid (2TMS)]	36	0.584	0.817	6,999	0.528	18	123	32	109	9	38 original
5855	51 [499; 2-Ethyl-3-hydroxy- 31 [626; 5-Methylthioadenosine (3TMS)]	38	0.582	0.889	6,628	0.524	19	122	25	116	8	40 original
13037	51 [499; 2-Ethyl-3-hydroxy- 32 [728; N,N-Dimethyllysine methyl ester]	44	0.581	0.862	16,044	0.834	20	121	6	135	41	2 duplicate
5813	51 [499; 2-Ethyl-3-hydroxy- 89 [775; Dopamine (4TMS)]	29	0.571	0.728	12,598	0.524	21	120	20	121	23	39 original
15163	51 [499; 2-Ethyl-3-hydroxy- 45 Homocysteine	43	0.557	0.650	5,834	0.538	22	119	29	112	3	32 duplicate
5791	51 [499; 2-Ethyl-3-hydroxy- 67 Clitic acid	44	0.550	0.688	35,620	0.512	23	118	26	115	119	47 original
10945	51 [499; 2-Ethyl-3-hydroxy- 8 Isoleucine	41	0.520	0.537	29,462	0.545	24	117	39	102	105	29 duplicate
13728	51 [499; 2-Ethyl-3-hydroxy- 31 [622; Parabenic acid (2TMS)]	44	0.503	0.819	13,445	0.535	25	116	12	129	30	33 duplicate
5819	51 [499; 2-Ethyl-3-hydroxy- 95 [770; 3,4,6-Trisubstitutedphenylmethanolamine (5TMS)]	38	0.491	0.540	6,225	0.513	26	115	38	103	5	46 original
11077	51 [499; 2-Ethyl-3-hydroxy- 9 Proline	44	0.490	0.718	39,674	0.586	27	114	22	119	122	12 duplicate
5776	51 [499; 2-Ethyl-3-hydroxy- 52 [NA]	31	0.475	0.494	10,679	0.565	28	113	40	101	15	21 original
14052	51 [499; 2-Ethyl-3-hydroxy- 34 Aspartic acid	44	0.446	0.694	44,701	0.577	29	112	24	117	135	16 duplicate
12820	51 [499; 2-Ethyl-3-hydroxy- 33 Homoserine	44	0.410	0.789	21,560	0.615	30	111	19	122	77	5 duplicate
5784	51 [499; 2-Ethyl-3-hydroxy- 60 Glycerol-3-phosphate	44	0.408	0.587	33,940	0.465	31	110	35	106	115	79 original
5787	51 [499; 2-Ethyl-3-hydroxy- 63 Glutamine	33	0.405	0.573	17,741	0.476	32	109	34	107	53	77 original
15537	51 [499; 2-Ethyl-3-hydroxy- 49 [877; Pyrophosphoric acid (4TMS)]	44	0.404	0.478	11,179	0.416	33	108	42	98	17	96 duplicate
12463	20 [619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	28	0.386	0.647	6,611	0.608	34	107	30	111	7	6 duplicate
5832	108 Octadecenoic acid	44	0.355	0.485	16,041	0.396	35	106	41	100	40	104 original
5822	51 [499; 2-Ethyl-3-hydroxy- 98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	35	0.355	0.801	5,106	0.608	36	105	16	125	2	7 original
10132	51 [499; 2-Ethyl-3-hydroxy- 2 Serine	44	0.351	0.707	30,608	0.573	37	104	23	118	107	17 duplicate
10812	51 [499; 2-Ethyl-3-hydroxy- 7 Threonine	44	0.330	0.626	41,328	0.540	38	103	31	110	127	31 duplicate
5780	51 [499; 2-Ethyl-3-hydroxy- 66 Glyceral acid-3-phosphate	44	0.328	0.615	16,419	0.508	39	102	33	108	45	50 original
14870	51 [499; 2-Ethyl-3-hydroxy- 43 [548; Leucine (2TBS)]	44	0.230	0.448	20,601	0.430	40	101	43	98	72	93 duplicate
5785	51 [499; 2-Ethyl-3-hydroxy- 71 [731; Erythrose (3TMS)]	44	0.228	0.286	25,411	0.485	41	100	49	92	90	67 original
14263	51 [499; 2-Ethyl-3-hydroxy- 36 [596; N-Acetylglutamic acid (2TMS)]	44	0.211	0.551	39,630	0.489	42	99	37	104	121	63 duplicate
5831	51 [499; 2-Ethyl-3-hydroxy- 107 9-(Z)-Octadecenoic acid	44	0.199	0.302	27,249	0.333	43	98	48	93	97	128 original
5789	51 [499; 2-Ethyl-3-hydroxy- 75 Lysine	44	0.182	0.553	49,531	0.499	44	97	36	105	138	54 original
5843	51 [499; 2-Ethyl-3-hydroxy- 119 [931; myo-Inositol-2-phosphate (7TMS)]	44	0.169	0.166	20,279	0.356	45	96	52	89	67	122 original
5848	124 [734; 1-Monooctadecyglycerol (2TMS); 1-Monohexadecyglycerol (1TMS)]	40	0.154	0.166	7,247	0.371	46	95	51	90	10	117 original
13282	51 [499; 2-Ethyl-3-hydroxy- 27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	41	0.144	0.685	11,941	0.624	47	94	27	114	19	3 duplicate
5814	51 [499; 2-Ethyl-3-hydroxy- 90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	44	0.140	0.099	19,860	0.335	48	93	53	88	63	125 original
5817	51 [499; 2-Ethyl-3-hydroxy- 93 [607; Putrescine (4TMS)]	42	0.134	-0.316	13,187	0.434	49	92	68	73	29	91 original
5854	51 [499; 2-Ethyl-3-hydroxy- 130 Trehalose	43	0.123	0.307	40,271	0.313	50	91	47	94	124	130 original
5835	51 [499; 2-Ethyl-3-hydroxy- 111 [583; Erythritol (4TMS)]	27	0.083	0.066	6,153	0.345	51	90	56	85	4	123 original
5861	51 [499; 2-Ethyl-3-hydroxy- 137 Ergosterol	44	0.070	0.235	25,969	0.385	52	89	50	91	92	114 original
5808	51 [499; 2-Ethyl-3-hydroxy- 84 Mannitol	44	0.057	-0.403	39,210	0.491	53	88	74	67	120	62 original
5777	51 [499; 2-Ethyl-3-hydroxy- 53 Glycerol-2-phosphate	44	0.047	0.071	12,332	0.320	54	87	55	86	21	127 original
10407	51 [499; 2-Ethyl-3-hydroxy- 4 Phosphoric acid	40	0.023	0.413	43,674	0.367	55	86	44	97	131	110 duplicate
5782	51 [499; 2-Ethyl-3-hydroxy- 58 [636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	44	-0.002	0.378	29,099	0.497	56	85	45	96	104	55 original
5865	51 [499; 2-Ethyl-3-hydroxy- 141 Lanosta-8,24-dien-3-beta-ol	43	-0.014	-0.090	11,375	0.357	57	84	60	81	18	121 original
5833	51 [499; 2-Ethyl-3-hydroxy- 109 Octadecanoic acid	44	-0.025	-0.363	32,957	0.444	58	83	72	69	111	87 original
5788	51 [499; 2-Ethyl-3-hydroxy- 64 [789; Tyramine (3TMS)]	43	-0.025	-0.051	17,332	0.361	59	82	59	82	49	119 original
5818	51 [499; 2-Ethyl-3-hydroxy- 94 Hexadecanoic acid	44	-0.027	-0.277	33,217	0.415	60	81	67	74	112	97 original
5863	51 [499; 2-Ethyl-3-hydroxy- 139 [700; Ergosta-5,7-dien-3-ol]	26	-0.028	0.081	6,519	0.316	61	80	54	87	6	128 original

5796	51	[499; 2-Ethyl-3-hydroxy-72 [919; D-Xylopyranose (4TMS)]	44	-0.070	0.008	16.625	0.294	62	79	57	84	46	134	original
5859	51	[499; 2-Ethyl-3-hydroxy-135	44	-0.074	-0.319	25.223	0.487	63	78	70	71	88	65	original
5862	51	[499; 2-Ethyl-3-hydroxy-138 [902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	31	-0.084	-0.127	8.765	0.393	64	77	61	80	13	108	original
5807	51	[499; 2-Ethyl-3-hydroxy-83 Sorbitol	43	-0.105	0.332	32.822	0.482	65	76	46	95	110	80	original
11848	51	[499; 2-Ethyl-3-hydroxy-15 Alanine	44	-0.106	-0.232	31.026	0.551	66	75	66	75	108	23	Juplicate
5864	51	[499; 2-Ethyl-3-hydroxy-140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	35	-0.116	-0.144	8.210	0.388	67	74	62	79	12	118	original
5836	51	[499; 2-Ethyl-3-hydroxy-112 [677; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	44	-0.140	-0.439	9.105	0.483	68	73	79	62	14	68	original
5857	51	[499; 2-Ethyl-3-hydroxy-133 [855; Squalene]	44	-0.152	-0.025	20.126	0.395	69	72	58	83	66	107	original
5820	51	[499; 2-Ethyl-3-hydroxy-96 myo-Inositol	36	-0.162	-0.200	7.588	0.269	70	71	64	77	11	138	original
5840	51	[499; 2-Ethyl-3-hydroxy-116 [882; Pseudouridine (5TMS)]	23	-0.162	-0.185	12.987	0.179	71	70	63	78	27	140	original
5788	51	[499; 2-Ethyl-3-hydroxy-74 [912; Tetradecanoic acid (1TMS)]	44	-0.197	-0.453	18.710	0.520	72	69	80	61	58	42	original
5803	51	[499; 2-Ethyl-3-hydroxy-79 Glucose	44	-0.216	-0.430	44.119	0.443	73	68	78	63	134	89	original
5824	51	[499; 2-Ethyl-3-hydroxy-100 [857; Mannitol (6TMS)]	44	-0.228	-0.558	22.004	0.443	74	67	91	50	78	88	original
5826	51	[499; 2-Ethyl-3-hydroxy-102 [904; Galactose methoxyamine (5TMS)]	44	-0.235	-0.409	16.368	0.480	75	66	75	68	44	72	original
5844	51	[499; 2-Ethyl-3-hydroxy-120 [945; Uridine (3TMS)]	36	-0.251	-0.224	23.089	0.494	76	65	65	76	84	58	original
12220	51	[499; 2-Ethyl-3-hydroxy-18 [590; 1-Acetyl-2-thichydantoin]	44	-0.254	-0.321	20.494	0.385	77	64	71	70	71	112	Juplicate
5809	51	[499; 2-Ethyl-3-hydroxy-85 [528; Methylcitric acid (4TMS)]	39	-0.258	-0.540	15.323	0.506	78	63	88	55	36	51	original
11467	51	[499; 2-Ethyl-3-hydroxy-12 Glyceric acid	43	-0.269	-0.674	12.809	0.472	79	62	107	34	26	78	Juplicate
5852	51	[499; 2-Ethyl-3-hydroxy-128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	27	-0.271	-0.497	19.334	0.294	80	61	83	58	61	135	original
15352	51	[499; 2-Ethyl-3-hydroxy-47 [NA]	44	-0.288	-0.318	20.372	0.339	81	60	69	72	69	124	Juplicate
5828	51	[499; 2-Ethyl-3-hydroxy-104 [795; Erythritol (4TMS)]	44	-0.292	-0.391	18.630	0.458	82	59	73	68	57	82	original
5851	51	[499; 2-Ethyl-3-hydroxy-127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	21	-0.314	-0.467	16.258	0.214	83	58	81	60	43	139	original
9993	51	[499; 2-Ethyl-3-hydroxy-1 [938; Sulfuric acid (2TMS)]	16	-0.317	-0.641	14.559	0.308	84	57	99	42	33	132	Juplicate
5815	51	[499; 2-Ethyl-3-hydroxy-91 [766; beta-D-Methylglucopyranoside (4TMS)]	44	-0.317	-0.548	22.895	0.514	85	56	89	52	82	45	original
5837	51	[499; 2-Ethyl-3-hydroxy-113 Galactose-6-phosphate	43	-0.318	-0.531	17.323	0.384	86	55	85	56	48	115	original
5838	51	[499; 2-Ethyl-3-hydroxy-114 Fructose-6-phosphate	35	-0.341	-0.543	15.687	0.359	87	54	87	54	38	120	original
5847	51	[499; 2-Ethyl-3-hydroxy-123 [945; Galactofuranose-6-phosphate (7TMS)]	44	-0.342	-0.418	24.207	0.433	88	53	76	65	86	92	original
5821	51	[499; 2-Ethyl-3-hydroxy-97 [756; beta-D-Methylglucopyranoside (4TMS)]	32	-0.351	-0.655	28.111	0.372	89	52	102	39	100	116	original
12583	51	[499; 2-Ethyl-3-hydroxy-21 [678; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	44	-0.362	-0.547	28.102	0.495	90	51	88	53	99	58	Juplicate
5842	51	[499; 2-Ethyl-3-hydroxy-118 [928; Glucopyranose-6-phosphate (6TMS)]	39	-0.387	-0.429	18.110	0.317	91	50	77	64	55	128	original
5850	51	[499; 2-Ethyl-3-hydroxy-126 [559; Erythritol (4TMS)]	27	-0.390	-0.528	15.898	0.448	92	49	84	57	39	85	original
10678	51	[499; 2-Ethyl-3-hydroxy-6 Glycerol	44	-0.397	-0.581	49.727	0.386	93	48	92	49	139	111	Juplicate
13168	51	[499; 2-Ethyl-3-hydroxy-28 Citramalic acid	44	-0.402	-0.602	28.638	0.520	94	47	93	48	102	41	Juplicate
15067	51	[499; 2-Ethyl-3-hydroxy-44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	30	-0.416	-0.811	19.625	0.395	95	46	94	47	62	106	Juplicate
11338	51	[499; 2-Ethyl-3-hydroxy-11 Succinic acid	44	-0.425	-0.647	20.652	0.419	96	45	101	40	74	95	Juplicate
13395	51	[499; 2-Ethyl-3-hydroxy-28 Malic acid	44	-0.429	-0.733	22.297	0.551	97	44	117	24	79	24	Juplicate
5829	51	[499; 2-Ethyl-3-hydroxy-105 [705; 2-Ketogluconic acid (5TMS)]	28	-0.439	-0.695	20.369	0.395	98	43	110	31	68	105	original
12702	51	[499; 2-Ethyl-3-hydroxy-22 [690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	36	-0.444	-0.755	12.091	0.477	99	42	123	18	20	75	Juplicate
5827	51	[499; 2-Ethyl-3-hydroxy-103 [648; Ethylamine (2TMS)]	43	-0.449	-0.872	22.572	0.504	100	41	108	35	81	52	original
5839	51	[499; 2-Ethyl-3-hydroxy-115 Glucose-6-phosphate	43	-0.453	-0.845	35.375	0.422	101	40	100	41	118	94	original
13507	51	[499; 2-Ethyl-3-hydroxy-29 Erythritol	44	-0.455	-0.780	17.574	0.535	102	39	127	14	51	34	Juplicate
5825	51	[499; 2-Ethyl-3-hydroxy-101 [832; Dopamine (4TMS)]	44	-0.457	-0.683	20.612	0.535	103	38	108	33	73	35	original
5797	51	[499; 2-Ethyl-3-hydroxy-73 [708; Glucose methoxyamine (5TMS)]	43	-0.468	-0.660	18.016	0.485	104	37	103	38	54	66	original
5849	51	[499; 2-Ethyl-3-hydroxy-125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	23	-0.469	-0.819	40.485	0.396	105	36	96	45	126	103	original
5823	51	[499; 2-Ethyl-3-hydroxy-99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	24	-0.478	-0.742	15.309	0.388	106	34	118	23	35	109	original
5856	51	[499; 2-Ethyl-3-hydroxy-132 [895; Isomaltose methoxyamine (8TMS)]	44	-0.482	-0.711	43.810	0.503	108	33	114	27	133	53	Juplicate
14673	51	[499; 2-Ethyl-3-hydroxy-40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	44	-0.486	-0.822	24.705	0.452	109	32	90	51	87	84	Juplicate
12342	51	[499; 2-Ethyl-3-hydroxy-19 Alanine (BP) (3TMS)	43	-0.488	-0.822	16.963	0.398	110	31	97	44	47	102	original
5802	51	[499; 2-Ethyl-3-hydroxy-71 Mannose	44	-0.499	-0.497	26.610	0.448	111	28	82	59	95	86	Juplicate
14773	51	[499; 2-Ethyl-3-hydroxy-41 [639; Proline (2TMS)]	44	-0.499	-0.497	26.610	0.448	111	28	82	59	95	86	Juplicate

14158	51 [499; 2-Ethyl-3-hydroxy-]	35	Pyroglutamic acid	44	-0.499	-0.666	49,276	0.453	112	29	104	37	137	83	duplicate
11722	51 [499; 2-Ethyl-3-hydroxy-]	14	Fumaric acid	44	-0.499	-0.749	14,165	0.549	113	30	121	20	32	28	duplicate
5800	51 [499; 2-Ethyl-3-hydroxy-]	76	Fructose	44	-0.507	-0.708	34,943	0.459	114	27	112	29	116	81	original
5816	51 [499; 2-Ethyl-3-hydroxy-]	92	[680; Glycerol-2-phosphate (4TMS)]	34	-0.508	-0.614	18,972	0.276	115	26	95	46	60	138	original
5778	51 [499; 2-Ethyl-3-hydroxy-]	54	[NA]	35	-0.509	-0.696	15,378	0.300	116	25	111	30	37	133	original
14470	51 [499; 2-Ethyl-3-hydroxy-]	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	44	-0.518	-0.821	20,487	0.479	117	24	132	9	70	73	duplicate
14572	51 [499; 2-Ethyl-3-hydroxy-]	39	[828; 1-Phenylethanol (1TMS)]	43	-0.522	-0.827	25,482	0.482	118	23	134	7	91	69	duplicate
5841	51 [499; 2-Ethyl-3-hydroxy-]	117	[724; Glycerol (3TMS)]	37	-0.535	-0.732	17,429	0.479	119	22	115	26	50	74	original
12097	51 [499; 2-Ethyl-3-hydroxy-]	17	[700; 2-methyl-1,2-propanediol (2TMS)]	44	-0.535	-0.746	26,567	0.442	120	21	120	21	101	90	duplicate
11973	51 [499; 2-Ethyl-3-hydroxy-]	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	44	-0.537	-0.830	28,891	0.527	121	20	135	6	103	37	duplicate
12837	51 [499; 2-Ethyl-3-hydroxy-]	24	[725; 2-Ketocacetic acid (2TMS)]	44	-0.550	-0.848	40,340	0.512	122	19	137	4	125	48	duplicate
5760	51 [499; 2-Ethyl-3-hydroxy-]	56	[828; Oxalic acid (3TMS)]	44	-0.558	-0.816	18,555	0.481	123	17	131	10	56	70	original
5858	51 [499; 2-Ethyl-3-hydroxy-]	134	Isomaltose	44	-0.556	-0.832	33,301	0.514	124	18	138	5	113	44	original
5789	51 [499; 2-Ethyl-3-hydroxy-]	65	[646; 3-Deoxyglucitol (5TMS)]	43	-0.557	-0.814	20,072	0.492	125	16	130	11	65	61	original
5846	51 [499; 2-Ethyl-3-hydroxy-]	122	[644; Erythritol (4TMS)]	32	-0.560	-0.752	14,718	0.413	126	15	122	19	34	98	original
5834	51 [499; 2-Ethyl-3-hydroxy-]	110	[715; Erythritol (4TMS)]	34	-0.561	-0.732	17,597	0.480	127	14	116	25	52	71	original
5804	51 [499; 2-Ethyl-3-hydroxy-]	80	[772; D-Glucose (5TMS)]	44	-0.562	-0.632	40,208	0.404	128	13	98	43	123	99	original
5784	51 [499; 2-Ethyl-3-hydroxy-]	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	43	-0.568	-0.669	30,514	0.399	129	12	105	38	106	101	original
5830	51 [499; 2-Ethyl-3-hydroxy-]	106	[733; Threitol (4TMS)]	42	-0.575	-0.766	21,298	0.545	130	11	124	17	75	28	original
15258	51 [499; 2-Ethyl-3-hydroxy-]	46	Arabinose	44	-0.575	-0.809	26,444	0.510	131	9	129	12	93	49	duplicate
5812	51 [499; 2-Ethyl-3-hydroxy-]	88	Glucuronic acid	44	-0.575	-0.850	23,340	0.550	132	10	138	3	85	25	original
5781	51 [499; 2-Ethyl-3-hydroxy-]	757	[757; 2-Desoxy-pentose-3-Mose dimethoxyamine (2TMS)]	35	-0.580	-0.773	22,924	0.385	133	8	125	18	83	113	original
5810	51 [499; 2-Ethyl-3-hydroxy-]	86	[793; D-Galactono-1,4-lactone (4TMS)]	42	-0.584	-0.779	28,091	0.532	134	7	126	15	98	38	original
5786	51 [499; 2-Ethyl-3-hydroxy-]	62	[812; D-Xylofuranose (4TMS)]	44	-0.586	-0.745	26,581	0.487	135	6	119	22	94	64	original
5853	51 [499; 2-Ethyl-3-hydroxy-]	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	39	-0.590	-0.827	20,024	0.493	136	5	133	8	64	60	original
5845	51 [499; 2-Ethyl-3-hydroxy-]	121	[657; Erythritol (4TMS)]	35	-0.593	-0.887	12,696	0.477	137	4	109	32	24	76	original
11595	51 [499; 2-Ethyl-3-hydroxy-]	13	Uracil	44	-0.609	-0.855	27,022	0.540	138	3	139	2	86	30	duplicate
5811	51 [499; 2-Ethyl-3-hydroxy-]	87	[945; beta-D-Glucopyranose (5TMS)]	44	-0.638	-0.708	43,699	0.401	139	2	113	28	132	100	original
15628	51 [499; 2-Ethyl-3-hydroxy-]	50	[746; Ribonic acid-1,4-lactone (3TMS)]	41	-0.676	-0.867	11,016	0.494	140	1	140	1	16	57	duplicate
5881	52 [NA]	68	[570; Hypoxanthine (2TMS)]	19	0.825	0.943	8,763	0.581	1	140	3	138	6	52	original
5876	52 [NA]	63	Glutamine	41	0.763	0.960	10,651	0.645	2	139	2	139	11	20	original
5902	52 [NA]	89	[775; Dopamine (4TMS)]	27	0.721	0.980	5,198	0.647	3	138	1	140	2	18	original
5868	52 [NA]	55	[612; 4-Aminobutyric acid (2TBS)]	27	0.613	0.921	6,144	0.688	4	137	5	136	3	4	original
10544	52 [NA]	5	Leucine	28	0.593	0.543	11,801	0.574	5	136	19	122	18	55	duplicate
5908	52 [NA]	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	39	0.530	0.673	8,487	0.544	6	135	12	129	4	71	original
15446	52 [NA]	48	Asparagine	46	0.511	0.722	18,452	0.646	7	134	9	132	51	19	duplicate
5918	52 [NA]	105	[705; 2-Ketogluconic acid (5TMS)]	30	0.490	0.794	25,094	0.593	8	133	7	134	85	42	original
15719	52 [NA]	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	31	0.475	0.494	10,679	0.585	9	132	23	118	13	60	duplicate
5874	52 [NA]	61	[NA]	46	0.474	0.689	17,940	0.691	10	131	10	131	47	78	original
5895	52 [NA]	82	Lysine	26	0.465	0.657	19,741	0.691	11	130	6	135	61	3	original
5944	52 [NA]	131	[626; 5-Methylthioadenosine (3TMS)]	40	0.464	0.768	8,746	0.607	12	129	8	133	5	34	original
5932	52 [NA]	119	[831; myo-Inositol-2-phosphate (7TMS)]	46	0.405	0.675	18,621	0.472	13	128	11	130	52	98	original
12464	52 [NA]	20	[619; 2-(3',4'-Bisubstitutedphenyl)-2-oxoethylamine (4TMS)]	23	0.368	0.938	4,537	0.693	14	127	4	137	1	2	duplicate
11209	52 [NA]	10	Glycine	46	0.362	0.844	28,376	0.685	15	126	13	128	99	16	duplicate
15538	52 [NA]	49	[877; Pyrophosphoric acid (4TMS)]	46	0.360	0.602	10,441	0.441	16	125	14	127	10	116	duplicate
5882	52 [NA]	69	Arginine	42	0.345	0.520	28,366	0.644	17	124	21	120	98	21	original
5903	52 [NA]	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	46	0.335	0.554	19,090	0.450	18	123	18	123	57	109	original
5920	52 [NA]	107	9-(Z)-Octadecenoic acid	46	0.333	0.579	25,912	0.384	19	121	17	124	91	131	original

13619	52 [NA]	30	[815; Ethyl-3-(2H)-thiophenone]	46	0.333	0.342	37,105	0.475	20	122	36	105	123	96 duplicate
10271	52 [NA]	45	Ethanolamine	45	0.331	0.590	12,641	0.685	21	120	15	128	23	5 duplicate
5890	52 [NA]	44	benzeneacetic acid methyl ester	44	0.317	0.460	35,951	0.523	22	119	24	117	120	79 original
5880	52 [NA]	46	Citric acid	46	0.314	0.513	33,669	0.533	23	118	22	119	115	76 original
15164	52 [NA]	43	Homocysteine	43	0.309	0.432	10,876	0.436	24	117	28	113	14	120 duplicate
13946	52 [NA]	46	Methionine	46	0.308	0.374	18,969	0.447	25	116	33	108	55	112 duplicate
5906	52 [NA]	43	[607; Putrescine (4TMS)]	43	0.305	0.168	13,391	0.494	26	115	49	92	26	90 original
14368	52 [NA]	46	Phenylalanine	46	0.300	0.441	32,580	0.565	27	114	26	115	113	59 duplicate
5894	52 [NA]	46	Tyrosine	46	0.299	0.583	40,626	0.704	28	113	16	125	130	1 original
14053	52 [NA]	46	Aspartic acid	46	0.295	0.321	40,534	0.442	29	112	41	100	129	115 duplicate
5911	52 [NA]	35	[697; Ribose-5-phosphate methoxyamine (5TMS)]	35	0.291	0.460	9,852	0.515	30	111	25	116	8	82 original
13729	52 [NA]	46	[622; Parabanic acid (2TMS)]	46	0.287	0.361	13,220	0.460	31	110	35	108	24	102 duplicate
5941	52 [NA]	30	[824; D-Sedoheptulose-7-phosphate (7TMS)]	30	0.283	0.035	22,105	0.566	32	109	59	82	74	58 original
14873	52 [NA]	43	Glutamic acid	43	0.282	0.390	34,650	0.494	33	108	30	111	116	81 duplicate
5873	52 [NA]	46	Glycerol-3-phosphate	46	0.277	0.534	30,914	0.608	34	107	20	121	111	32 original
8994	52 [NA]	25	[938; Sulfuric acid (2TMS)]	25	0.273	0.151	16,234	0.583	35	106	52	89	41	51 duplicate
10946	52 [NA]	37	Isoleucine	37	0.267	0.173	25,315	0.404	36	105	48	93	87	128 duplicate
5921	52 [NA]	46	Octadecanoic acid	46	0.264	0.391	15,777	0.356	37	104	29	112	37	136 original
12821	52 [NA]	46	Homoserine	46	0.233	0.438	18,865	0.531	38	103	27	114	53	77 duplicate
5940	52 [NA]	28	[777; Fructose-6-phosphate methoxyamine (6TMS)]	28	0.233	0.375	17,320	0.477	39	102	32	109	46	95 original
5950	52 [NA]	46	Ergosterol	46	0.212	0.268	24,171	0.361	40	101	73	88	118	134 original
5910	52 [NA]	34	[756; beta-D-Methylglucopyranoside (4TMS)]	34	0.209	-0.280	35,092	0.637	41	100	43	98	79	23 original
5866	52 [NA]	46	Glycerol-2-phosphate	46	0.186	0.337	13,447	0.453	42	99	37	104	27	106 original
13838	52 [NA]	45	[729; N,N-Dimethyllysine methyl ester]	45	0.182	0.365	14,870	0.592	43	98	34	107	30	43 duplicate
11078	52 [NA]	9	Proline	45	0.172	0.199	33,457	0.428	44	97	46	95	114	123 duplicate
5954	52 [NA]	141	Lanosta-8,24-dien-3-beta-ol	43	0.169	0.376	11,845	0.455	45	96	31	110	19	104 original
5872	52 [NA]	59	Ornithine; Arginine	46	0.163	0.327	47,442	0.516	46	95	40	101	138	81 original
10813	52 [NA]	7	Threonine	46	0.159	0.195	38,620	0.420	47	94	47	94	126	125 duplicate
5884	52 [NA]	71	[731; Erythrose (3TMS)]	46	0.157	0.162	24,008	0.454	48	93	50	91	78	105 original
5937	52 [NA]	124	[734; 1-Monocoleglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	42	0.141	0.329	12,347	0.359	49	92	39	102	21	135 original
10133	52 [NA]	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	30	0.117	-0.345	15,209	0.606	50	91	80	61	33	35 original
5897	52 [NA]	2	Serine	44	0.114	0.153	25,840	0.418	51	90	51	90	90	126 duplicate
13283	52 [NA]	84	Mannitol	44	0.110	0.006	42,153	0.625	52	89	61	80	132	28 original
13054	52 [NA]	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	37	0.108	0.330	13,315	0.556	53	88	38	103	25	65 duplicate
5870	52 [NA]	25	[709; 2,5-Diaminovalerolactam (2TMS)]	31	0.088	0.201	14,222	0.543	54	87	45	96	28	73 duplicate
5867	52 [NA]	57	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	37	0.078	-0.562	27,597	0.574	55	86	101	40	95	56 original
5939	52 [NA]	54	[NA]	37	0.075	-0.435	18,334	0.585	56	85	88	53	50	49 original
5952	52 [NA]	128	[559; Erythritol (4TMS)]	28	0.074	-0.119	16,105	0.628	57	84	70	71	39	27 original
5907	52 [NA]	139	[700; Ergosta-5,7-dien-3-ol]	28	0.069	0.296	10,006	0.396	58	83	42	99	9	129 original
5878	52 [NA]	94	Hexadecanoic acid	46	0.067	-0.105	30,702	0.501	59	82	68	73	110	86 original
5895	52 [NA]	66	Glyceric acid-3-phosphate	46	0.051	0.120	16,219	0.507	60	81	55	86	40	84 original
15068	52 [NA]	72	[919; D-Xylopyranose (4TMS)]	45	0.051	0.131	16,525	0.293	61	80	53	88	43	136 original
5929	52 [NA]	44	[910; 2-Ketoglucuronic acid methoxyamine (4TMS)]	32	0.040	-0.294	21,764	0.598	62	79	75	66	69	39 duplicate
14971	52 [NA]	116	[862; Pseudouridine (5TMS)]	20	0.032	0.256	11,157	0.351	63	78	44	97	16	137 original
14264	52 [NA]	43	[548; Leucine (2TBS)]	42	0.031	0.020	19,379	0.556	64	77	60	81	59	68 duplicate
5922	52 [NA]	36	[596; N-Acetylglutamic acid (2TMS)]	46	0.024	0.126	36,722	0.478	65	76	54	87	121	94 duplicate
5924	52 [NA]	109	Octadecanoic acid	46	-0.005	-0.301	30,495	0.495	66	75	76	65	107	89 original
		111	[583; Erythritol (4TMS)]	28	-0.005	-0.114	9,054	0.257	67	74	69	72	7	139 original

5905	52 [NA]	92 [880; Glycerol-2-phosphate (4TMS)]	36 -0.006	-0.706	21.962	0.554	68	73	122	19	72	68 original
5942	52 [NA]	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	41 -0.034	-0.553	24.418	0.633	69	72	99	42	80	25 original
5948	52 [NA]	135	46 -0.053	-0.167	24.589	0.440	70	71	72	69	82	117 original
5949	52 [NA]	[802; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	9 -0.056	-0.391	10.672	0.112	71	70	85	56	12	140 original
5953	52 [NA]	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	35 -0.066	0.053	11.092	0.427	72	69	58	85	15	124 original
5909	52 [NA]	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	34 -0.073	0.053	12.162	0.381	73	68	57	84	20	132 original
5943	52 [NA]	96 myo-inositol	45 -0.089	0.051	38.682	0.442	74	67	58	83	127	114 original
15353	52 [NA]	130 Trehalose	46 -0.094	-0.084	21.554	0.469	75	68	68	75	68	99 duplicate
11468	52 [NA]	47 [NA]	45 -0.095	-0.368	15.203	0.458	76	65	83	58	32	103 duplicate
5935	52 [NA]	12 Glyceral acid	34 -0.098	-0.361	15.885	0.581	77	64	82	59	38	53 original
12703	52 [NA]	122 [644; Erythritol (4TMS)]	36 -0.098	-0.352	14.955	0.560	78	63	81	60	31	63 duplicate
5925	52 [NA]	22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	46 -0.105	-0.335	12.558	0.513	79	62	78	63	22	83 original
5988	52 [NA]	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	46 -0.107	0.003	46.228	0.461	80	61	62	79	137	101 original
5986	52 [NA]	75 Lysine	40 -0.113	-0.010	26.896	0.434	81	60	63	78	102	121 original
5933	52 [NA]	83 Sorbitol	39 -0.117	-0.282	25.588	0.556	82	59	74	67	88	64 original
5951	52 [NA]	120 [945; Uridine (3TMS)]	34 -0.130	-0.104	11.190	0.453	83	58	67	74	17	107 original
13508	52 [NA]	138 [674; Ergosterol (1TMS)]	46 -0.130	-0.511	18.668	0.589	84	57	96	45	54	45 duplicate
10408	52 [NA]	29 Erythritol	33 -0.133	-0.015	37.756	0.451	85	56	64	77	125	108 duplicate
5945	52 [NA]	4 Phosphoric acid	28 -0.138	-0.439	15.522	0.533	86	55	89	52	35	75 original
11974	52 [NA]	132 [895; Isomaltose methoxyamine (8TMS)]	46 -0.154	-0.562	30.638	0.680	87	54	102	39	109	8 duplicate
15259	52 [NA]	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	46 -0.157	-0.896	31.523	0.674	88	53	120	21	112	8 duplicate
14573	52 [NA]	46 Arabinose	45 -0.158	-0.549	29.858	0.618	89	52	98	43	105	30 duplicate
5915	52 [NA]	39 [829; 1-Phenylethanol (1TMS)]	46 -0.161	-0.330	17.107	0.449	90	51	77	64	44	110 original
15629	52 [NA]	102 [904; Galactose methoxyamine (5TMS)]	43 -0.163	-0.493	14.758	0.564	91	50	94	47	29	61 duplicate
5878	52 [NA]	50 [746; Ribonic acid-1,4-lactone (3TMS)]	45 -0.166	-0.665	25.270	0.668	92	49	115	26	86	13 original
5913	52 [NA]	65 [646; 3-Deoxyglucitol (5TMS)]	46 -0.181	-0.336	22.096	0.447	93	48	79	62	73	111 original
5923	52 [NA]	100 [857; Mannitol (6TMS)]	36 -0.184	-0.592	20.189	0.652	94	47	109	32	63	17 original
		110 [715; Erythritol (4TMS)]										
		58 [636; 4R-Acetamido-2,3-(2-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	46 -0.186	-0.064	26.411	0.438	95	45	65	76	93	119 original
5871	52 [NA]	24 [725; 2-Ketocetonic acid (2TMS)]	46 -0.186	-0.614	42.293	0.685	96	46	110	31	133	6 duplicate
12838	52 [NA]	88 Gluconic acid	46 -0.189	-0.569	26.306	0.667	97	44	104	37	92	15 original
5901	52 [NA]	17 [700; 2-methyl-1,2-propanediol (2TMS)]	46 -0.194	-0.581	30.546	0.608	98	43	108	33	108	33 duplicate
12098	52 [NA]	56 [829; Orotic acid (3TMS)]	46 -0.210	-0.681	23.087	0.673	99	42	118	23	76	11 original
5869	52 [NA]	91 [766; beta-D-Methylglucopyranoside (4TMS)]	46 -0.225	-0.390	29.989	0.603	100	41	84	57	106	38 original
5904	52 [NA]	11 Succinic acid	46 -0.231	-0.621	21.797	0.586	101	40	112	29	70	49 duplicate
11339	52 [NA]	103 [648; Ethylamine (2TMS)]	45 -0.232	-0.498	28.268	0.597	102	39	95	46	97	40 original
5916	52 [NA]	134 Isomaltose	46 -0.233	-0.671	37.719	0.668	103	38	117	24	124	14 original
5947	52 [NA]	133 [855; Squalene]	46 -0.241	-0.152	19.369	0.394	104	37	71	70	58	130 original
5946	52 [NA]	85 [529; Methylcitric acid (4TMS)]	30 -0.251	-0.412	15.647	0.500	105	36	86	55	36	87 original
5998	52 [NA]	13 Ureil	46 -0.256	-0.577	29.838	0.672	106	35	108	35	104	12 duplicate
11596	52 [NA]	74 [912; Tetradecanoic acid (1TMS)]	46 -0.258	-0.415	18.972	0.475	107	34	87	54	56	97 original
5987	52 [NA]	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	46 -0.262	-0.579	21.903	0.587	108	33	107	34	71	47 duplicate
14471	52 [NA]	101 [832; Dopamine (4TMS)]	46 -0.268	-0.452	24.751	0.555	109	31	90	51	84	67 original
5914	52 [NA]	21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	46 -0.268	-0.483	28.635	0.482	110	32	92	49	100	93 duplicate
12584	52 [NA]	26 Citramalic acid	46 -0.285	-0.456	28.135	0.464	111	30	91	50	96	100 duplicate
13169	52 [NA]	86 [793; D-Galactono-1,4-lactone (4TMS)]	43 -0.287	-0.767	34.664	0.674	112	29	129	12	117	10 original
5899	52 [NA]	18 [590; 1-Acetyl-2-thiohydantoin]	46 -0.287	-0.484	20.870	0.431	113	28	93	48	66	122 duplicate
12221	52 [NA]	62 [812; D-Xylofuranose (4TMS)]	46 -0.306	-0.683	26.988	0.577	114	27	119	22	84	54 original
5975	52 [NA]	117 [724; Glycerol (3TMS)]	39 -0.317	-0.563	19.446	0.544	115	26	103	38	60	72 original

11723	52 [NA]	14 Fumaric acid	46 -0.320	-0.557	16.263	0.552	116	25	100	41	42	69 duplicate
13396	52 [NA]	28 Malic acid	46 -0.328	-0.577	22.735	0.585	117	24	105	36	75	50 duplicate
5934	52 [NA]	121 [657; Erythritol (4TMS)]	38 -0.331	-0.616	15.356	0.542	118	23	111	30	34	74 original
5931	52 [NA]	118 [928; Glucopyranose-6-phosphate (6TMS)]	41 -0.334	-0.519	18.307	0.378	119	22	97	44	49	133 original
5938	52 [NA]	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	46 -0.355	-0.872	41.596	0.596	120	21	135	6	131	41 original
5983	52 [NA]	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	40 -0.367	-0.670	28.868	0.442	121	20	116	25	101	113 original
5986	52 [NA]	73 [708; Glucose methoxyamine (5TMS)]	39 -0.374	-0.699	20.368	0.498	122	19	121	20	64	88 original
5928	52 [NA]	115 Glucose-6-phosphate	45 -0.376	-0.856	35.760	0.588	123	18	132	9	119	46 original
14674	52 [NA]	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	46 -0.376	-0.636	43.095	0.606	124	17	113	28	134	36 duplicate
5900	52 [NA]	76 [945; beta-D-Glucopyranose (5TMS)]	44 -0.376	-0.758	43.206	0.490	125	16	128	13	138	92 original
5989	52 [NA]	87 Fructose	46 -0.393	-0.846	36.767	0.592	126	15	131	10	122	44 original
14159	52 [NA]	35 Pyroglutamic acid	46 -0.399	-0.841	48.721	0.614	127	14	130	11	139	31 duplicate
5977	52 [NA]	64 [788; Tyramine (3TMS)]	45 -0.414	-0.661	18.037	0.413	128	12	114	27	48	127 original
5991	52 [NA]	78 Mannose	45 -0.414	-0.716	21.305	0.502	129	13	124	17	87	85 original
11949	52 [NA]	108 [733; Threitol (4TMS)]	46 -0.443	-0.739	24.547	0.684	130	11	126	15	81	7 original
10679	52 [NA]	15 Alanine	46 -0.507	-0.878	29.721	0.605	131	10	138	5	103	37 duplicate
5993	52 [NA]	8 Glycerol	46 -0.509	-0.868	49.287	0.550	132	9	134	7	140	70 duplicate
5993	52 [NA]	80 [772; D-Glucose (5TMS)]	45 -0.517	-0.756	39.535	0.439	133	8	127	14	128	118 original
14774	52 [NA]	41 [639; Proline (2TMS)]	46 -0.530	-0.707	25.637	0.518	134	7	123	18	89	80 duplicate
5917	52 [NA]	104 [795; Erythritol (4TMS)]	45 -0.533	-0.730	20.757	0.561	135	6	125	16	65	62 original
5926	52 [NA]	113 Galactose-6-phosphate	45 -0.554	-0.908	19.931	0.627	136	5	138	3	62	26 original
12343	52 [NA]	19 Alanine (BP) (3TMS)	46 -0.614	-0.860	24.686	0.573	137	4	133	8	83	57 duplicate
5927	52 [NA]	114 Fructose-6-phosphate	40 -0.618	-0.904	17.217	0.624	138	3	137	4	45	29 original
5936	52 [NA]	123 [945; Galactofuranose-6-phosphate (7TMS)]	46 -0.648	-0.910	23.624	0.638	139	2	139	2	77	22 original
5992	52 [NA]	79 Glucose	46 -0.697	-0.940	43.193	0.634	140	1	140	1	135	24 original
12485	53 Glycerol-2-phosphate	20 [619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	31 0.553	0.669	8.841	0.465	1	140	1	140	21	1 duplicate
6000	53 Glycerol-2-phosphate	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41 0.339	0.367	7.383	0.429	2	139	7	134	7	7 original
9995	53 Glycerol-2-phosphate	1 [938; Sulfuric acid (2TMS)]	36 0.327	0.494	8.404	0.377	3	138	3	138	17	48 duplicate
5964	53 Glycerol-2-phosphate	63 Glutamine	52 0.305	0.313	13.642	0.361	4	137	11	130	65	71 original
5990	53 Glycerol-2-phosphate	89 [775; Dopamine (4TMS)]	35 0.304	0.487	12.603	0.341	5	136	4	137	51	105 original
6032	53 Glycerol-2-phosphate	131 [626; 5-Methylthiadenosine (3TMS)]	55 0.255	0.503	7.782	0.408	6	135	2	139	12	16 original
5991	53 Glycerol-2-phosphate	90 [910; 9-(2)-Hexadecenoic acid (1TMS)]	64 0.254	0.314	11.285	0.393	7	134	10	131	38	31 original
5983	53 Glycerol-2-phosphate	82 Lysine	39 0.252	0.379	20.102	0.383	8	133	6	135	93	41 original
5998	53 Glycerol-2-phosphate	97 [756; beta-D-Methylglucopyranoside (4TMS)]	52 0.240	0.395	25.809	0.377	9	132	5	136	108	49 original
5994	53 Glycerol-2-phosphate	93 [607; Putrescine (4TMS)]	60 0.228	0.249	9.350	0.359	10	131	16	125	26	74 original
6030	53 Glycerol-2-phosphate	129 [940; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	59 0.200	0.175	14.492	0.367	11	130	23	118	75	36 original
15354	53 Glycerol-2-phosphate	47 [NA]	64 0.196	0.328	12.856	0.378	12	129	9	132	60	47 duplicate
15630	53 Glycerol-2-phosphate	50 [746; Ribonic acid-1,4-lactone (3TMS)]	61 0.191	0.179	10.065	0.355	13	128	22	119	34	83 duplicate
6008	53 Glycerol-2-phosphate	107 9-(2)-Octadecenoic acid	64 0.186	0.252	20.063	0.362	14	127	15	126	92	69 original
15809	53 Glycerol-2-phosphate	52 [NA]	46 0.186	0.337	13.447	0.453	15	126	8	133	64	3 duplicate
5985	53 Glycerol-2-phosphate	84 Mannitol	62 0.174	0.289	37.379	0.389	16	125	13	128	128	34 original
5958	53 Glycerol-2-phosphate	757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55 0.169	-0.008	18.383	0.367	17	124	46	95	87	61 original
15539	53 Glycerol-2-phosphate	49 [877; Pyrophosphoric acid (4TMS)]	64 0.156	0.305	12.929	0.340	18	123	12	129	61	106 duplicate
6020	53 Glycerol-2-phosphate	119 [931; myo-Inositol-2-phosphate (7TMS)]	64 0.151	0.147	12.054	0.405	19	122	26	115	48	17 original
6006	53 Glycerol-2-phosphate	105 [705; 2-Ketogluconic acid (5TMS)]	48 0.138	0.284	15.960	0.379	20	121	14	127	80	45 original
6031	53 Glycerol-2-phosphate	130 Trehalose	63 0.132	0.229	36.124	0.344	21	120	19	122	125	88 original
6021	53 Glycerol-2-phosphate	120 [945; Uridine (3TMS)]	54 0.131	0.232	17.221	0.357	22	119	18	123	83	79 original
10545	53 Glycerol-2-phosphate	5 Leucine	45 0.123	0.208	9.181	0.332	23	118	20	121	24	115 duplicate

13055	53 Glycerol-2-phosphate	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	0,101	-0,002	13,118	0,352	24	117	44	97	63	89 duplicate
6009	53 Glycerol-2-phosphate	108	Octadecanoic acid	64	0,100	0,122	7,409	0,364	25	116	29	112	8	68 original
6025	53 Glycerol-2-phosphate	124	[734; 1-Monooleoylglycerol (1TMS)]	59	0,099	0,088	14,362	0,400	26	115	33	108	72	21 original
6029	53 Glycerol-2-phosphate	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0,095	0,032	12,955	0,330	27	114	37	104	62	118 original
5955	53 Glycerol-2-phosphate	54	[NA]	55	0,077	-0,030	9,962	0,311	28	113	49	92	31	133 original
11597	53 Glycerol-2-phosphate	13	Uracil	64	0,074	0,004	22,095	0,401	29	112	43	98	97	18 duplicate
5956	53 Glycerol-2-phosphate	55	[612; 4-Aminobutyric acid (2TBS)]	63	0,074	0,236	14,413	0,352	30	111	17	124	73	87 original
5973	53 Glycerol-2-phosphate	72	[919; D-Xylopyranose (4TMS)]	63	0,069	0,132	8,879	0,330	31	110	28	113	22	117 original
5962	53 Glycerol-2-phosphate	61	[NA]	64	0,063	-0,020	9,746	0,321	32	109	48	93	29	125 original
5966	53 Glycerol-2-phosphate	65	[646; 3-Deoxyglucitol (5TMS)]	63	0,060	-0,059	15,604	0,376	33	108	62	79	78	51 original
6035	53 Glycerol-2-phosphate	134	Isomaltose	64	0,059	-0,057	31,317	0,366	34	107	60	81	118	62 original
5987	53 Glycerol-2-phosphate	86	[793; D-Galactono-1,4-lactone (4TMS)]	61	0,052	-0,129	27,347	0,358	35	106	79	62	111	76 original
16447	53 Glycerol-2-phosphate	48	Asparagine	64	0,052	-0,018	8,602	0,408	37	105	47	94	19	15 duplicate
13509	53 Glycerol-2-phosphate	29	Erythritol	64	0,052	-0,018	8,602	0,408	37	105	47	94	19	15 duplicate
14972	53 Glycerol-2-phosphate	43	[548; Leucine (2TBS)]	60	0,047	0,207	11,658	0,353	38	103	21	120	41	86 duplicate
15720	53 Glycerol-2-phosphate	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	0,047	0,071	12,332	0,320	39	102	35	106	50	126 duplicate
15260	53 Glycerol-2-phosphate	46	Arabinose	64	0,044	-0,086	22,936	0,371	40	101	67	74	100	55 duplicate
14574	53 Glycerol-2-phosphate	39	[829; 1-Phenylethanol (1TMS)]	63	0,040	-0,033	21,836	0,356	41	100	52	89	95	80 duplicate
5993	53 Glycerol-2-phosphate	92	[680; Glycerol-2-phosphate (4TMS)]	54	0,036	-0,065	11,723	0,318	42	99	63	78	42	128 original
5992	53 Glycerol-2-phosphate	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	0,035	0,145	20,304	0,355	43	97	27	114	94	82 original
12939	53 Glycerol-2-phosphate	24	[725; beta-D-Ketooctanoic acid (2TMS)]	64	0,035	-0,042	38,494	0,401	44	98	55	86	130	19 duplicate
6028	53 Glycerol-2-phosphate	127	[777; Fructose-6-phosphate methoxamine (6TMS)]	39	0,034	0,020	8,801	0,294	45	96	39	102	20	137 original
5957	53 Glycerol-2-phosphate	56	[829; Oroic acid (3TMS)]	64	0,032	-0,090	12,736	0,365	46	95	68	73	66	65 original
5989	53 Glycerol-2-phosphate	88	Gluconic acid	64	0,028	0,016	17,209	0,400	47	94	40	101	82	20 original
12089	53 Glycerol-2-phosphate	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	0,026	-0,057	23,628	0,350	48	93	61	80	101	91 duplicate
6040	53 Glycerol-2-phosphate	139	[700; Ergosta-5,7-dien-3-ol]	38	0,024	0,004	10,409	0,314	49	92	42	99	35	130 original
12704	53 Glycerol-2-phosphate	22	[690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0,023	0,021	7,246	0,310	50	91	38	103	5	134 duplicate
14874	53 Glycerol-2-phosphate	42	Glutamic acid	60	0,020	-0,127	35,369	0,333	51	90	78	63	122	113 duplicate
11975	53 Glycerol-2-phosphate	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	0,015	-0,034	23,808	0,425	52	89	53	88	103	8 duplicate
11469	53 Glycerol-2-phosphate	12	Glyceric acid	63	0,012	-0,075	5,478	0,355	53	88	65	76	2	84 duplicate
6002	53 Glycerol-2-phosphate	101	[832; Dopamine (4TMS)]	64	0,003	0,104	14,595	0,358	54	87	30	111	77	77 original
6038	53 Glycerol-2-phosphate	137	Ergosterol	64	-0,003	-0,031	19,470	0,343	55	88	50	91	89	101 original
6023	53 Glycerol-2-phosphate	122	[644; Erythritol (4TMS)]	52	-0,008	0,008	11,391	0,349	56	85	41	100	39	92 original
11210	53 Glycerol-2-phosphate	10	Glycine	64	-0,012	0,051	24,623	0,395	57	84	36	105	107	38 duplicate
5970	53 Glycerol-2-phosphate	69	Arginine	60	-0,014	-0,005	26,663	0,335	58	83	45	96	109	110 original
5988	53 Glycerol-2-phosphate	87	[945; beta-D-Glucopyranose (5TMS)]	62	-0,014	-0,051	41,483	0,362	59	82	57	84	136	70 original
12622	53 Glycerol-2-phosphate	23	Homoserine	64	-0,015	0,096	13,887	0,344	60	80	31	110	66	89 duplicate
5975	53 Glycerol-2-phosphate	74	[912; Tetradecanoic acid (1TMS)]	64	-0,015	-0,317	12,714	0,444	61	81	124	17	64	6 original
6042	53 Glycerol-2-phosphate	141	Lanosta-8,24-dien-3-beta-ol	61	-0,015	-0,056	7,563	0,419	62	79	59	82	10	12 original
14054	53 Glycerol-2-phosphate	34	Aspartic acid	64	-0,017	-0,101	39,072	0,339	63	78	73	68	131	108 duplicate
10947	53 Glycerol-2-phosphate	8	Isoleucine	55	-0,020	-0,091	23,717	0,325	64	77	69	72	102	122 duplicate
6004	53 Glycerol-2-phosphate	103	[648; Ethylamine (2TMS)]	63	-0,020	0,078	18,480	0,374	65	76	34	107	88	52 original
14472	53 Glycerol-2-phosphate	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0,024	-0,104	12,616	0,329	66	75	74	67	52	119 duplicate
5963	53 Glycerol-2-phosphate	62	[812; D-Xylofuranose (4TMS)]	64	-0,026	-0,066	19,820	0,360	67	74	64	77	91	72 original
11724	53 Glycerol-2-phosphate	14	Fumaric acid	64	-0,027	-0,094	5,476	0,350	68	73	70	71	1	90 duplicate
5960	53 Glycerol-2-phosphate	59	Ornithine; Arginine	64	-0,028	-0,123	47,364	0,328	69	72	77	64	138	120 original
14875	53 Glycerol-2-phosphate	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0,029	-0,097	40,837	0,356	70	71	71	70	134	81 duplicate
5999	53 Glycerol-2-phosphate	98	[697; Ribose-5-phosphate methoxamine (5TMS)]	48	-0,030	0,161	11,879	0,373	71	70	24	117	46	53 original
5995	53 Glycerol-2-phosphate	94	Hexadecanoic acid	64	-0,031	-0,339	27,933	0,464	72	69	129	12	113	2 original
12585	53 Glycerol-2-phosphate	21	[678; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	64	-0,036	-0,117	22,482	0,346	73	68	75	66	99	97 duplicate

6010	53 Glycerol-2-phosphate	109 Octadecanoic acid	64 -0.038	-0.361	28.648	0.384	74	67	130	11	114	39 original
6026	53 Glycerol-2-phosphate	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64 -0.044	-0.199	38.413	0.368	75	66	96	45	129	60 original
10680	53 Glycerol-2-phosphate	8 Glycerol	64 -0.046	-0.175	48.279	0.355	76	65	91	50	140	85 duplicate
13284	53 Glycerol-2-phosphate	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53 -0.049	0.086	14.182	0.311	77	64	32	109	69	132 duplicate
11340	53 Glycerol-2-phosphate	11 Succinic acid	64 -0.053	-0.155	12.676	0.359	78	63	84	57	53	73 duplicate
13620	53 Glycerol-2-phosphate	30 [815; Ethyl-3(2H)-thiophenone]	64 -0.058	-0.138	36.015	0.357	79	62	81	60	124	78 duplicate
6034	53 Glycerol-2-phosphate	133 [855; Squalene]	64 -0.057	-0.187	11.888	0.383	80	81	88	53	47	40 original
13397	53 Glycerol-2-phosphate	28 Malic acid	64 -0.070	-0.130	14.483	0.342	81	60	80	61	74	103 duplicate
15165	53 Glycerol-2-phosphate	45 Homocysteine	61 -0.071	-0.034	12.822	0.312	82	59	54	87	58	131 duplicate
13947	53 Glycerol-2-phosphate	33 Methionine	64 -0.071	-0.082	14.250	0.335	83	58	66	75	71	111 duplicate
6027	53 Glycerol-2-phosphate	126 [559; Erythritol (4TMS)]	45 -0.075	-0.216	9.374	0.387	84	57	100	41	27	35 original
13730	53 Glycerol-2-phosphate	31 [622; Parabenic acid (2TMS)]	64 -0.075	-0.052	6.362	0.320	85	56	58	83	3	127 duplicate
13170	53 Glycerol-2-phosphate	26 Citramalic acid	64 -0.082	-0.155	22.162	0.327	86	55	85	56	98	121 duplicate
10409	53 Glycerol-2-phosphate	4 Phosphoric acid	51 -0.084	-0.191	39.137	0.282	87	54	94	47	132	138 duplicate
6013	53 Glycerol-2-phosphate	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63 -0.089	-0.236	7.849	0.411	88	53	107	34	11	14 original
14265	53 Glycerol-2-phosphate	36 [596; N-Acetylglutamic acid (2TMS)]	64 -0.092	-0.228	34.969	0.370	89	52	105	36	121	57 duplicate
5986	53 Glycerol-2-phosphate	85 [529; Methylcitric acid (4TMS)]	48 -0.096	-0.271	8.255	0.378	90	51	118	23	15	46 original
5982	53 Glycerol-2-phosphate	81 Tyrosine	64 -0.098	-0.121	40.270	0.422	91	50	76	65	133	11 original
5979	53 Glycerol-2-phosphate	78 Mannose	62 -0.097	-0.187	11.788	0.323	92	49	93	48	44	124 original
5996	53 Glycerol-2-phosphate	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50 -0.100	-0.149	12.818	0.395	93	48	83	58	57	27 original
13839	53 Glycerol-2-phosphate	32 [729; N,N-Dimethyllysine methyl ester]	63 -0.104	-0.169	14.187	0.378	94	47	89	52	70	44 duplicate
10272	53 Glycerol-2-phosphate	3 Ebanolamine	62 -0.104	-0.098	7.874	0.397	95	46	72	69	13	22 duplicate
6001	53 Glycerol-2-phosphate	100 [857; Mannitol (6TMS)]	64 -0.105	-0.166	13.959	0.333	96	45	87	54	67	112 original
6041	53 Glycerol-2-phosphate	140 [892; Ergosta-7,22-dien-3-ol (1TMS)]	49 -0.105	-0.182	8.087	0.429	97	44	95	46	14	8 original
6033	53 Glycerol-2-phosphate	132 [895; Isomaltose methoxyamine (8TMS)]	42 -0.106	-0.033	12.315	0.271	98	43	51	90	49	139 original
5978	53 Glycerol-2-phosphate	77 [826; beta-[[[5-methyl-2-thienyl)methyl]eneamino-benzeneacetic acid methyl ester]	62 -0.106	-0.210	35.799	0.331	99	42	99	42	123	116 original
5981	53 Glycerol-2-phosphate	80 [772; D-Glucose (5TMS)]	62 -0.112	-0.048	36.814	0.394	100	41	56	85	127	28 original
5987	53 Glycerol-2-phosphate	66 Glycemic acid-3-phosphate	64 -0.121	-0.200	7.472	0.324	101	40	97	44	9	123 original
6007	53 Glycerol-2-phosphate	106 [733; Threitol (4TMS)]	62 -0.123	-0.177	15.672	0.348	102	39	92	49	79	85 original
5968	53 Glycerol-2-phosphate	67 Clitic acid	64 -0.127	-0.220	29.940	0.342	103	38	101	40	116	104 original
5959	53 Glycerol-2-phosphate	58 [636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64 -0.128	-0.228	21.900	0.359	104	37	104	37	98	75 original
5977	53 Glycerol-2-phosphate	76 Fructose	64 -0.130	-0.228	31.983	0.366	105	36	106	35	119	84 original
11079	53 Glycerol-2-phosphate	9 Proline	63 -0.137	-0.241	33.415	0.349	106	35	110	31	120	93 duplicate
14160	53 Glycerol-2-phosphate	35 Pyrogulamic acid	64 -0.138	-0.255	47.842	0.380	107	34	113	28	139	43 duplicate
15069	53 Glycerol-2-phosphate	44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	50 -0.138	-0.240	14.505	0.316	108	33	108	33	76	129 duplicate
12222	53 Glycerol-2-phosphate	18 [590; 1-Acetyl-2-thiohydantoin]	64 -0.139	-0.314	12.729	0.347	109	32	123	18	55	96 duplicate
5976	53 Glycerol-2-phosphate	75 Lysine	64 -0.141	-0.260	46.158	0.366	110	31	115	26	137	63 original
6022	53 Glycerol-2-phosphate	121 [657; Erythritol (4TMS)]	55 -0.146	-0.224	9.040	0.369	111	30	102	39	23	59 original
5971	53 Glycerol-2-phosphate	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57 -0.152	-0.263	24.289	0.352	112	29	116	25	105	88 original
6018	53 Glycerol-2-phosphate	117 [724; Glycerol (3TMS)]	56 -0.160	-0.225	11.211	0.376	113	28	103	38	37	50 original
6011	53 Glycerol-2-phosphate	110 [715; Erythritol (4TMS)]	54 -0.164	-0.263	12.823	0.417	114	27	117	24	59	13 original
6003	53 Glycerol-2-phosphate	102 [904; Galactose methoxyamine (5TMS)]	64 -0.165	-0.283	7.357	0.337	115	26	121	20	6	109 original
6036	53 Glycerol-2-phosphate	135 [902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64 -0.170	-0.327	17.740	0.394	116	25	126	15	85	29 original
14369	53 Glycerol-2-phosphate	37 Phenylalanine	64 -0.172	-0.284	28.915	0.363	117	24	119	22	115	68 duplicate
10134	53 Glycerol-2-phosphate	2 Serine	62 -0.172	-0.240	24.148	0.349	118	23	109	32	104	94 duplicate
5037	53 Glycerol-2-phosphate	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17 -0.176	-0.253	6.970	0.213	119	22	111	30	4	140 original
5980	53 Glycerol-2-phosphate	79 Glucose	64 -0.179	-0.253	41.455	0.364	120	21	112	29	135	67 original
6005	53 Glycerol-2-phosphate	104 [795; Erythritol (4TMS)]	63 -0.185	-0.203	11.484	0.390	121	20	98	43	40	33 original



6019	53 Glycerol-2-phosphate	118 [928; Glucopyranose-6-phosphate (6TMS)]	58 -0.192	-0.285	9.903	0.393	122	19	120	21	30	30 original
5974	53 Glycerol-2-phosphate	73 [708; Glucose methoxyamine (5TMS)]	57 -0.197	-0.256	11.828	0.333	123	18	114	27	45	114 original
6016	53 Glycerol-2-phosphate	115 Glucose-6-phosphate	62 -0.203	-0.333	31.129	0.392	124	17	127	14	117	32 original
6039	53 Glycerol-2-phosphate	138 [674; Ergosterol (1TMS)]	46 -0.214	-0.469	9.509	0.451	125	16	140	1	28	4 original
10814	53 Glycerol-2-phosphate	7 Threonine	64 -0.217	-0.294	36.511	0.343	126	15	122	19	128	102 duplicate
11850	53 Glycerol-2-phosphate	15 Alanine	64 -0.227	-0.327	24.598	0.369	127	13	125	18	106	58 duplicate
14775	53 Glycerol-2-phosphate	41 [639; Proline (2TMS)]	64 -0.227	-0.366	19.581	0.425	128	14	132	9	80	10 duplicate
5965	53 Glycerol-2-phosphate	64 [789; Tyramine (3TMS)]	63 -0.235	-0.371	8.278	0.370	129	12	134	7	16	56 original
12344	53 Glycerol-2-phosphate	19 Alanine (BP) (3TMS)	64 -0.236	-0.363	17.753	0.445	130	11	131	10	88	5 duplicate
5961	53 Glycerol-2-phosphate	60 Glycerol-3-phosphate	64 -0.242	-0.370	27.635	0.395	131	10	133	8	112	28 original
6017	53 Glycerol-2-phosphate	116 [882; Pseudouridine (5TMS)]	30 -0.269	-0.449	9.188	0.297	132	9	82	59	25	136 original
5972	53 Glycerol-2-phosphate	71 [731; Erythrose (3TMS)]	64 -0.289	-0.469	17.711	0.372	133	8	139	2	84	54 original
5997	53 Glycerol-2-phosphate	98 myo-Inositol	49 -0.289	-0.173	11.144	0.395	134	7	90	51	36	25 original
6024	53 Glycerol-2-phosphate	123 [945; Galactofuranose-6-phosphate (7TMS)]	64 -0.313	-0.388	16.418	0.387	135	6	135	6	81	37 original
6015	53 Glycerol-2-phosphate	114 Fructose-6-phosphate	53 -0.313	-0.418	8.531	0.380	136	5	137	4	18	42 original
5984	53 Glycerol-2-phosphate	83 Sorbitol	62 -0.320	-0.403	10.059	0.396	137	4	138	5	33	24 original
5969	53 Glycerol-2-phosphate	68 [570; Hypoxanthine (2TMS)]	58 -0.337	-0.334	26.915	0.301	138	3	128	13	110	135 original
6012	53 Glycerol-2-phosphate	111 [583; Erythritol (4TMS)]	20 -0.347	-0.157	10.036	0.344	139	2	86	55	32	100 original
11976	54 [NA]	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	42 -0.350	-0.423	11.740	0.339	140	1	138	3	43	107 original
6044	54 [NA]	56 [829; Orotic acid (3TMS)]	55 -0.780	0.934	22.037	0.596	1	140	6	135	102	18 duplicate
12940	54 [NA]	24 [725; 2-Ketobutanoic acid (2TMS)]	55 0.785	0.960	6.611	0.638	2	139	1	140	7	2 original
15261	54 [NA]	46 Arabinose	55 0.782	0.938	35.941	0.618	3	138	5	136	129	9 duplicate
		57	55 0.770	0.952	18.578	0.626	4	137	2	139	88	7 duplicate
6045	54 [NA]	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	51 0.765	0.932	12.553	0.662	5	136	7	134	46	1 original
6122	54 [NA]	134 Isomaltose	55 0.762	0.947	28.391	0.628	6	135	3	138	116	6 original
11598	54 [NA]	13 Uracil	55 0.760	0.924	20.010	0.578	7	134	9	132	93	30 duplicate
6053	54 [NA]	65 [646; 3-Deoxyglucitol (5TMS)]	54 0.755	0.942	8.156	0.628	8	133	4	137	13	5 original
6050	54 [NA]	62 [812; D-Xylofuranose (4TMS)]	55 0.752	0.917	19.192	0.611	9	132	11	130	90	13 original
11341	54 [NA]	21 Succinic acid	55 0.723	0.896	12.528	0.605	10	131	14	127	45	16 duplicate
13510	54 [NA]	29 Erythritol	55 0.717	0.903	9.690	0.580	11	130	13	128	26	28 duplicate
6117	54 [NA]	129 [940; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	52 0.715	0.923	8.945	0.604	12	129	10	131	23	17 original
6076	54 [NA]	88 Gluconic acid	55 0.714	0.873	14.975	0.606	13	128	18	123	66	15 original
6074	54 [NA]	86 [793; D-Galactono-1,4-lactone (4TMS)]	52 0.710	0.932	22.975	0.610	14	127	8	133	103	14 original
12100	54 [NA]	17 [700; 2-methyl-1,2-propanediol (2TMS)]	55 0.701	0.886	21.649	0.542	15	126	17	124	101	48 duplicate
14575	54 [NA]	39 [829; 1-Phenylethanol (1TMS)]	54 0.684	0.891	18.130	0.572	16	125	15	126	84	33 duplicate
15931	54 [NA]	50 [746; Ribonic acid-1,4-lactone (3TMS)]	54 0.682	0.871	9.458	0.560	17	124	19	122	24	41 duplicate
11470	54 [NA]	12 Glycine acid	55 0.647	0.826	6.533	0.540	18	123	23	118	6	49 duplicate
12705	54 [NA]	22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	46 0.629	0.853	4.840	0.551	19	122	22	119	3	46 duplicate
6080	54 [NA]	92 [680; Glycerol-2-phosphate (4TMS)]	52 0.618	0.788	7.679	0.522	20	121	29	112	11	55 original
11725	54 [NA]	14 Fumaric acid	55 0.616	0.857	7.100	0.579	21	120	21	120	9	29 duplicate
6087	54 [NA]	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	38 0.616	0.910	3.696	0.635	22	119	12	129	1	3 original
8996	54 [NA]	1 [938; Sulfuric acid (2TMS)]	38 0.616	0.754	5.037	0.592	23	118	35	108	5	21 duplicate
14473	54 [NA]	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	55 0.609	0.889	12.057	0.630	24	117	16	125	40	4 duplicate
13398	54 [NA]	28 Malic acid	55 0.589	0.857	14.385	0.536	25	116	20	121	62	52 duplicate
6091	54 [NA]	103 [648; Ethylamine (2TMS)]	54 0.580	0.762	15.078	0.474	26	115	33	108	68	71 original
6093	54 [NA]	105 [705; 2-Ketogluconic acid (5TMS)]	48 0.534	0.792	11.212	0.559	27	114	28	113	35	43 original
12586	54 [NA]	21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	55 0.518	0.711	21.388	0.526	28	113	37	104	98	54 duplicate
6100	54 [NA]	112 [677; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	54 0.514	0.694	10.435	0.474	29	112	41	100	29	72 original
6058	54 [NA]	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	48 0.511	0.521	23.821	0.491	30	111	58	83	105	66 original

6113	54 [NA]	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	55	0.507	0.785	36.470	0.562	31	110	30	111	130	39 original
6104	54 [NA]	116 [882; Pseudouridine (5TMS)]	25	0.500	0.368	8.627	0.362	32	109	68	75	19	119 original
6085	54 [NA]	97 [756; beta-D-Methylglucopyranoside (4TMS)]	50	0.494	0.776	21.592	0.556	33	108	32	109	99	44 original
6116	54 [NA]	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.483	0.798	8.238	0.572	34	107	26	115	15	34 original
6090	54 [NA]	102 [904; Galactose methoxyamine (5TMS)]	55	0.471	0.733	8.661	0.507	35	106	36	105	20	59 original
6073	54 [NA]	85 [529; Methylcitric acid (4TMS)]	39	0.468	0.614	10.876	0.397	36	105	51	90	32	107 original
13171	54 [NA]	26 Citramalic acid	55	0.464	0.661	21.605	0.495	37	104	46	95	100	64 duplicate
6088	54 [NA]	100 [857; Mannitol (6TMS)]	55	0.455	0.761	13.560	0.528	38	103	34	107	56	53 original
6079	54 [NA]	91 [766; beta-D-Methylglucopyranoside (4TMS)]	55	0.452	0.673	17.009	0.398	39	102	43	98	74	106 original
6108	54 [NA]	120 [945; Uridine (3TMS)]	48	0.443	0.325	14.874	0.545	40	101	69	72	65	47 original
14161	54 [NA]	35 Pyroglutamic acid	55	0.433	0.820	45.014	0.575	41	99	24	117	139	32 duplicate
6089	54 [NA]	101 [832; Dopamine (4TMS)]	55	0.433	0.661	13.034	0.422	42	100	45	96	50	93 original
6103	54 [NA]	115 Glucose-6-phosphate	54	0.427	0.780	29.075	0.618	43	98	31	110	118	11 original
14676	54 [NA]	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	55	0.426	0.701	38.338	0.519	44	97	40	101	133	56 duplicate
6123	54 [NA]	135	55	0.418	0.585	17.697	0.474	45	96	53	88	81	73 original
6064	54 [NA]	902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	55	0.417	0.820	29.924	0.566	46	95	25	116	119	37 original
6066	54 [NA]	76 Fructose	53	0.406	0.701	8.594	0.516	47	94	39	102	18	58 original
6061	54 [NA]	73 [708; Glucose methoxyamine (5TMS)]	48	0.402	0.665	9.535	0.440	48	93	44	97	25	87 original
6120	54 [NA]	132 [895; Isomaltose methoxyamine (6TMS)]	41	0.385	0.795	8.685	0.594	49	92	27	114	21	20 original
6075	54 [NA]	87 [945; beta-D-Glucopyranose (5TMS)]	53	0.382	0.688	40.121	0.565	50	91	42	99	136	38 original
6072	54 [NA]	84 Mannitol	53	0.380	0.584	34.164	0.472	51	89	54	87	123	74 original
6094	54 [NA]	106 [733; Threitol (4TMS)]	53	0.379	0.704	13.383	0.571	52	89	38	103	55	35 original
6115	54 [NA]	127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.331	0.641	4.713	0.596	53	88	49	92	4	19 original
12223	54 [NA]	18 [590; 1-Acetyl-2-thiohydantoin]	55	0.293	0.458	13.299	0.379	54	87	61	80	54	116 duplicate
6081	54 [NA]	93 [607; Putrescine (4TMS)]	51	0.293	0.381	11.028	0.362	55	86	65	76	34	120 original
6082	54 [NA]	74 [912; Tetradecanoic acid (1TMS)]	55	0.262	0.437	11.594	0.391	56	85	62	79	36	110 original
6110	54 [NA]	122 [644; Erythritol (4TMS)]	49	0.252	0.639	8.738	0.561	57	84	50	91	22	40 original
6084	54 [NA]	96 myo-Inositol	40	0.244	0.231	12.007	0.307	58	83	73	68	38	136 original
6105	54 [NA]	117 [724; Glycerol (3TMS)]	49	0.226	0.559	8.406	0.502	59	82	55	86	16	82 original
6078	54 [NA]	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	55	0.224	0.117	12.974	0.418	60	81	80	61	49	98 original
15355	54 [NA]	47 [NA]	55	0.215	0.155	14.591	0.450	61	80	78	63	63	82 duplicate
6109	54 [NA]	121 [657; Erythritol (4TMS)]	48	0.215	0.478	8.045	0.540	62	79	60	81	12	50 original
6098	54 [NA]	110 [715; Erythritol (4TMS)]	49	0.206	0.545	8.227	0.625	63	78	56	85	14	8 original
15070	54 [NA]	44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	49	0.199	0.544	10.962	0.585	64	77	57	84	33	26 duplicate
10681	54 [NA]	6 Glycerol	55	0.185	0.594	45.588	0.537	65	76	52	89	140	51 duplicate
6101	54 [NA]	113 Galactose-6-phosphate	54	0.168	0.646	8.462	0.591	66	75	47	94	17	22 original
6051	54 [NA]	63 Glutamine	43	0.161	-0.522	17.154	0.617	67	74	106	35	76	12 original
6114	54 [NA]	126 [559; Erythritol (4TMS)]	45	0.149	0.356	7.384	0.585	68	73	67	74	10	25 original
12345	54 [NA]	19 Alanine (BP) (3TMS)	55	0.142	0.432	17.671	0.507	69	72	63	78	80	60 duplicate
6088	54 [NA]	80 [772; D-Glucose (5TMS)]	53	0.136	0.511	35.662	0.503	70	71	59	82	128	61 original
6099	54 [NA]	111 [583; Erythritol (4TMS)]	40	0.131	0.356	14.684	0.418	71	68	73	64	95	95 original
6128	54 [NA]	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	40	0.126	0.220	9.886	0.355	72	69	75	66	27	123 original
6071	54 [NA]	83 Sorbitol	49	0.114	-0.353	27.042	0.317	73	68	93	48	112	134 original
6102	54 [NA]	114 Fructose-6-phosphate	46	0.109	0.644	6.927	0.554	74	67	48	93	8	45 original
14776	54 [NA]	41 [639; Proline (2TMS)]	55	0.096	0.235	19.720	0.443	75	66	72	69	91	85 duplicate
15898	54 [NA]	53 Glycerol-2-phosphate	55	0.077	-0.030	9.962	0.311	76	65	82	59	28	135 duplicate
15810	54 [NA]	52 [NA]	37	0.075	-0.435	18.334	0.585	77	64	98	43	86	24 duplicate
6095	54 [NA]	107 9-(Z)-Octadecenoic acid	55	0.051	-0.177	20.060	0.435	78	63	90	51	94	88 original
6127	54 [NA]	139 [700; Ergosta-5,7-dien-3-ol]	31	0.049	-0.059	12.665	0.412	79	62	85	56	47	100 original
6107	54 [NA]	119 [931; myo-Inositol-2-phosphate (7TMS)]	55	0.046	-0.055	13.673	0.407	80	61	84	57	58	102 original

6129	54 [NA]	141	Lanoste-8,24-dien-3-beta-ol	52	0.039	0.065	10.862	0.339	81	60	81	60	31	131	original
6097	54 [NA]	109	Octadecanoic acid	55	0.020	0.180	27.222	0.401	82	59	77	64	113	105	original
6052	54 [NA]	64	[789; Tyramine (3TMS)]	55	0.009	0.302	10.777	0.374	83	57	70	71	30	117	original
6082	54 [NA]	94	Hexadecanoic acid	55	0.009	0.122	26.578	0.403	84	58	79	82	111	104	original
6092	54 [NA]	104	[795; Erythritol (4TMS)]	54	-0.001	0.228	12.900	0.458	85	56	74	67	48	80	original
6111	54 [NA]	123	[945; Galactofuranose-6-phosphate (7TMS)]	55	-0.003	0.261	17.023	0.483	86	55	71	70	75	68	original
6121	54 [NA]	133	[855; Squalene]	55	-0.010	-0.078	14.021	0.359	87	54	86	55	59	121	original
6125	54 [NA]	137	Ergosterol	55	-0.036	-0.161	19.869	0.348	88	53	87	54	92	127	original
11851	54 [NA]	15	Alanine	55	-0.052	0.193	24.418	0.559	89	52	76	65	106	42	duplicate
6060	54 [NA]	72	[919; D-Xylopyranose (4TMS)]	54	-0.059	-0.248	13.200	0.351	90	51	92	49	53	124	original
6049	54 [NA]	61	[NA]	55	-0.102	-0.164	12.075	0.441	91	50	88	53	41	88	original
6124	54 [NA]	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.103	-0.386	4.294	0.426	92	49	97	44	2	92	original
6059	54 [NA]	71	[731; Erythrose (3TMS)]	55	-0.107	-0.230	18.121	0.435	93	48	91	50	83	89	original
6126	54 [NA]	138	[674; Ergosterol (1TMS)]	38	-0.124	-0.035	12.045	0.390	94	47	83	58	39	111	original
6106	54 [NA]	118	[928; Glucopyranose-6-phosphate (6TMS)]	51	-0.183	-0.176	11.728	0.453	95	46	89	52	37	81	original
14973	54 [NA]	43	[548; Leucine (2TBS)]	51	-0.202	-0.355	15.077	0.351	96	45	94	47	67	125	duplicate
6096	54 [NA]	108	Octadecanoic acid	55	-0.213	-0.447	12.226	0.413	97	44	101	40	43	99	original
6112	54 [NA]	124	[734; 1-Monocleoylglycerol (2TMS); 1-Monohexadecenoylethanol (1TMS)]	50	-0.224	-0.382	17.502	0.411	98	43	95	46	79	101	original
6067	54 [NA]	79	Glucose	55	-0.238	0.402	39.676	0.818	99	42	64	77	135	10	original
15166	54 [NA]	45	Homocysteine	52	-0.268	-0.386	16.528	0.350	100	41	96	45	72	126	duplicate
15540	54 [NA]	49	[877; Pyrophosphoric acid (4TMS)]	55	-0.285	-0.438	18.339	0.444	101	40	99	42	87	84	duplicate
13056	54 [NA]	25	[709; 2,5-Diaminovalerolactam (2TMS)]	47	-0.297	-0.815	18.695	0.581	102	39	133	8	89	27	duplicate
6088	54 [NA]	98	[697; Ribose-5-phosphate methoxymine (5TMS)]	40	-0.313	-0.691	16.906	0.415	103	38	123	18	73	98	original
10815	54 [NA]	7	Threonine	55	-0.333	-0.486	34.521	0.344	104	37	102	39	125	129	duplicate
6077	54 [NA]	89	[775; Dopamine (4TMS)]	26	-0.335	-0.796	17.432	0.459	105	36	131	10	77	79	original
10410	54 [NA]	4	Phosphoric acid	43	-0.340	-0.503	38.610	0.290	106	35	104	37	134	138	duplicate
12923	54 [NA]	23	Homoserine	55	-0.359	-0.734	18.245	0.491	107	34	125	16	85	67	duplicate
6118	54 [NA]	130	Trehalose	55	-0.371	-0.446	34.755	0.340	108	33	100	41	127	130	original
6055	54 [NA]	67	Citric acid	55	-0.378	-0.562	28.516	0.394	109	32	109	32	117	108	original
6119	54 [NA]	131	[626; 5-Methylthioadenosine (3TMS)]	47	-0.382	-0.539	13.616	0.466	110	31	107	34	57	76	original
6048	54 [NA]	60	Glycerol-3-phosphate	55	-0.385	-0.559	26.484	0.470	111	30	108	33	110	75	original
14370	54 [NA]	37	Phenylalanine	55	-0.401	-0.616	27.689	0.394	112	29	115	26	115	115	duplicate
14055	54 [NA]	34	Aspartic acid	55	-0.402	-0.509	36.857	0.418	113	28	105	36	131	94	duplicate
6083	54 [NA]	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	41	-0.410	-0.582	16.122	0.339	114	27	111	30	70	132	original
15448	54 [NA]	48	Asparagine	55	-0.421	-0.738	17.501	0.570	115	26	126	15	78	38	duplicate
13285	54 [NA]	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	44	-0.444	-0.759	20.705	0.461	116	25	127	14	96	78	duplicate
6056	54 [NA]	68	[570; Hypoxanthine (2TMS)]	12	-0.455	-0.893	12.222	0.333	117	24	137	4	42	133	original
13948	54 [NA]	33	Methionine	55	-0.464	-0.590	17.831	0.432	118	23	112	29	82	90	duplicate
6054	54 [NA]	66	Glyceric acid-3-phosphate	55	-0.479	-0.629	12.400	0.404	119	21	116	25	44	103	original
14266	54 [NA]	36	[596; N-Acetylglutamic acid (2TMS)]	55	-0.479	-0.637	33.655	0.393	120	22	118	23	121	109	duplicate
10135	54 [NA]	2	Serine	53	-0.488	-0.630	26.093	0.358	121	20	117	24	109	122	duplicate
6046	54 [NA]	58	[636; 4R-Acetaldo-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	55	-0.491	-0.503	23.151	0.384	122	19	103	38	104	114	original
10948	54 [NA]	8	Isoleucine	46	-0.492	-0.578	25.639	0.280	123	18	110	31	108	140	duplicate
13621	54 [NA]	30	[815; Ethyl-3(2H)-thiophenone]	55	-0.494	-0.600	34.453	0.344	124	17	113	28	124	128	duplicate
6063	54 [NA]	75	Lysine	55	-0.500	-0.601	43.669	0.428	125	16	114	27	137	91	original
13731	54 [NA]	31	[622; Parabenic acid (2TMS)]	55	-0.502	-0.679	13.191	0.478	126	15	122	19	52	70	duplicate
15721	54 [NA]	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	35	-0.509	-0.696	15.378	0.300	127	14	124	17	69	137	duplicate
10546	54 [NA]	5	Leucine	36	-0.556	-0.660	14.223	0.285	128	13	119	22	61	139	duplicate
11080	54 [NA]	9	Proline	54	-0.563	-0.664	33.415	0.387	129	12	120	21	120	112	duplicate

6043	54 [NA]	55 [612; 4-Aminobutyric acid (2TBS)]	34 -0.569	-0.837	16,336	0.385	130	11	134	7	71	113 original
13840	54 [NA]	32 [728; N,N-Dimethyllysine methyl ester]	54 -0.584	-0.781	20,550	0.492	131	10	130	11	95	65 duplicate
6057	54 [NA]	69 Arginine	51 -0.586	-0.841	27,243	0.517	132	9	135	6	114	57 original
10273	54 [NA]	3 Ethanolamine	53 -0.591	-0.814	14,082	0.499	133	8	132	9	60	63 duplicate
6065	54 [NA]	77 [826; beta-[(5-methyl-2-thienyl)methyl]eneamino-benzeneacetic acid methyl ester]	53 -0.614	-0.765	34,067	0.369	134	7	129	12	122	118 original
6047	54 [NA]	59 Ornithine; Arginine	55 -0.631	-0.672	44,231	0.447	135	6	121	20	138	83 original
14875	54 [NA]	42 Glutamic acid	51 -0.633	-0.760	34,717	0.417	136	5	128	13	126	97 duplicate
12466	54 [NA]	20 [619; 2-(3'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	22 -0.654	-0.911	13,052	0.464	137	4	139	2	51	77 duplicate
6069	54 [NA]	81 Tyrosine	55 -0.665	-0.881	37,253	0.575	138	3	136	5	132	31 original
11211	54 [NA]	10 Glycine	55 -0.679	-0.906	24,560	0.588	139	2	138	3	107	23 duplicate
6070	54 [NA]	82 Lysine	30 -0.701	-0.932	20,985	0.483	140	1	140	1	97	69 original
6155	55 [612; 4-Aminobutyric acid]	81 Tyrosine	43 0.772	0.941	48,027	0.696	1	140	3	138	136	1 original
6142	55 [612; 4-Aminobutyric acid]	68 [570; Hypoxanthine (2TMS)]	14 0.738	0.989	3,538	0.609	2	139	1	140	1	11 original
11212	55 [612; 4-Aminobutyric acid]	10 Glycine	43 0.721	0.872	34,165	0.592	3	138	9	132	107	19 duplicate
15449	55 [612; 4-Aminobutyric acid]	48 Asparagine	43 0.714	0.849	23,193	0.619	4	137	10	131	75	8 duplicate
6163	55 [612; 4-Aminobutyric acid]	77 [775; Dopamine (4TMS)]	26 0.686	0.967	9,768	0.651	5	136	2	139	13	4 original
6151	55 [612; 4-Aminobutyric acid]	77 [826; beta-[(5-methyl-2-thienyl)methyl]eneamino-benzeneacetic acid methyl ester]	43 0.679	0.825	44,982	0.607	6	135	12	129	130	14 original
10274	55 [612; 4-Aminobutyric acid]	3 Ethanolamine	43 0.672	0.897	16,127	0.649	7	134	8	133	32	5 duplicate
6156	55 [612; 4-Aminobutyric acid]	82 Lysine	33 0.659	0.915	26,164	0.608	8	133	6	135	86	13 original
6169	55 [612; 4-Aminobutyric acid]	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	35 0.657	0.837	5,377	0.592	9	132	11	130	3	21 original
14876	55 [612; 4-Aminobutyric acid]	42 Glutamic acid	42 0.633	0.593	44,356	0.569	10	131	25	116	129	32 duplicate
15811	55 [612; 4-Aminobutyric acid]	52 [NA]	27 0.613	0.921	6,144	0.688	11	130	5	138	4	2 duplicate
10547	55 [612; 4-Aminobutyric acid]	5 Leucine	39 0.609	0.593	17,014	0.474	12	129	24	117	38	82 duplicate
6135	55 [612; 4-Aminobutyric acid]	61 [NA]	43 0.604	0.717	20,366	0.491	13	128	15	126	54	75 original
13622	55 [612; 4-Aminobutyric acid]	30 [815; Ethyl-3(2H)-thiophenone]	43 0.597	0.498	44,167	0.584	14	127	29	112	128	36 duplicate
6143	55 [612; 4-Aminobutyric acid]	69 Arginine	43 0.598	0.688	36,651	0.529	15	126	17	124	115	59 original
15722	55 [612; 4-Aminobutyric acid]	51 [899; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	36 0.584	0.617	6,999	0.526	16	125	23	118	5	60 duplicate
6137	55 [612; 4-Aminobutyric acid]	63 Glutamine	32 0.556	0.906	14,734	0.561	17	124	7	134	29	38 original
15541	55 [612; 4-Aminobutyric acid]	49 [877; Pyrophosphoric acid (4TMS)]	43 0.553	0.696	10,450	0.441	18	123	16	125	17	102 duplicate
6141	55 [612; 4-Aminobutyric acid]	67 Citric acid	43 0.550	0.749	37,594	0.521	19	122	13	128	119	63 original
6205	55 [612; 4-Aminobutyric acid]	131 [626; 5-Methylthioadenosine (3TMS)]	38 0.533	0.720	8,775	0.608	20	121	14	127	10	12 original
14371	55 [612; 4-Aminobutyric acid]	37 Phenylalanine	43 0.530	0.645	37,122	0.532	21	119	20	121	118	56 duplicate
13949	55 [612; 4-Aminobutyric acid]	33 Methionine	43 0.530	0.464	24,322	0.568	22	120	34	107	81	34 duplicate
6134	55 [612; 4-Aminobutyric acid]	60 Glycerol-3-phosphate	43 0.499	0.648	36,027	0.507	23	118	19	122	112	68 original
6133	55 [612; 4-Aminobutyric acid]	59 Ornithine; Arginine	43 0.488	0.666	53,131	0.565	24	117	18	123	140	35 original
12467	55 [612; 4-Aminobutyric acid]	20 [619; 2-(3'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	29 0.463	0.924	4,165	0.661	25	116	4	137	2	3 duplicate
15167	55 [612; 4-Aminobutyric acid]	45 Homocysteine	41 0.437	0.459	8,451	0.437	26	115	31	110	9	104 duplicate
6182	55 [612; 4-Aminobutyric acid]	108 Octadecenoic acid	43 0.420	0.558	18,261	0.385	27	114	26	115	40	119 original
6158	55 [612; 4-Aminobutyric acid]	84 Mannitol	42 0.415	0.465	36,730	0.485	28	113	33	108	116	79 original
13841	55 [612; 4-Aminobutyric acid]	32 [729; N,N-Dimethyllysine methyl ester]	43 0.398	0.519	19,854	0.556	29	112	28	113	46	42 duplicate
14056	55 [612; 4-Aminobutyric acid]	34 Aspartic acid	43 0.393	0.437	45,928	0.521	30	110	35	106	133	62 duplicate
10949	55 [612; 4-Aminobutyric acid]	8 Isoleucine	43 0.393	0.391	33,449	0.470	31	111	37	104	106	88 duplicate
13057	55 [612; 4-Aminobutyric acid]	25 [709; 2,5-Diaminovalerolactam (2TMS)]	28 0.349	0.484	20,916	0.472	32	109	30	111	59	83 duplicate
6167	55 [612; 4-Aminobutyric acid]	93 [607; Putrescine (4TMS)]	40 0.333	0.313	10,326	0.507	33	108	41	100	15	67 original
6193	55 [612; 4-Aminobutyric acid]	119 [931; myo-Inositol-2-phosphate (7TMS)]	43 0.318	0.640	21,142	0.488	34	107	21	120	61	76 original
11081	55 [612; 4-Aminobutyric acid]	9 Proline	43 0.307	0.410	43,123	0.594	35	106	36	105	125	18 duplicate
13732	55 [612; 4-Aminobutyric acid]	31 [622; Parabanic acid (2TMS)]	43 0.288	0.348	16,761	0.467	36	105	39	102	37	89 duplicate

12824	55 [612; 4-Aminobutyric acid]	23	Homoserine	43	0.267	0.468	24.803	0.533	37	104	32	109	84	55 duplicate
6181	55 [612; 4-Aminobutyric acid]	107	9-(Z)-Octadecanoic acid	43	0.262	0.622	28.923	0.426	38	103	22	119	97	108 original
6140	55 [612; 4-Aminobutyric acid]	66	Glyceric acid-3-phosphate	43	0.212	0.209	19.584	0.487	39	102	48	95	44	77 original
6164	55 [612; 4-Aminobutyric acid]	90	9-(10; 9-Z)-Hexadecanoic acid (1TMS)	43	0.209	0.557	21.099	0.470	40	101	27	114	60	87 original
6145	55 [612; 4-Aminobutyric acid]	71	[731; Erythrose (3TMS)]	43	0.147	0.136	27.751	0.467	41	100	49	92	90	90 original
6172	55 [612; 4-Aminobutyric acid]	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	32	0.145	0.300	9.358	0.558	42	99	43	98	11	41 original
6198	55 [612; 4-Aminobutyric acid]	124	[734; 1-Monooleoylglycerol (2TMS); 1-Monoheptadecanoylglycerol (1TMS)]	39	0.120	0.324	8.367	0.373	43	98	40	101	8	126 original
6211	55 [612; 4-Aminobutyric acid]	137	Ergosterol	43	0.118	0.350	28.097	0.433	44	97	38	103	94	108 original
10816	55 [612; 4-Aminobutyric acid]	7	Threonine	43	0.110	0.129	43.587	0.571	45	96	52	89	127	31 duplicate
10138	55 [612; 4-Aminobutyric acid]	2	Serine	43	0.103	0.139	34.346	0.597	46	95	48	93	110	16 duplicate
14974	55 [612; 4-Aminobutyric acid]	43	[548; Leucine (2TBS)]	42	0.087	0.135	22.706	0.464	47	94	50	91	70	92 duplicate
15899	55 [612; 4-Aminobutyric acid]	53	Glycerol-2-phosphate	43	0.074	0.236	14.413	0.352	48	93	45	96	26	130 duplicate
6215	55 [612; 4-Aminobutyric acid]	141	Larosta-8,24-dien-3-beta-ol	43	0.065	0.310	12.908	0.391	49	92	42	99	21	117 original
6148	55 [612; 4-Aminobutyric acid]	72	[919; D-Xylopyranose (4TMS)]	43	0.059	0.089	18.775	0.317	50	91	53	88	43	133 original
14267	55 [612; 4-Aminobutyric acid]	36	[598; N-Acetylglucamic acid (2TMS)]	43	0.045	0.135	43.202	0.544	51	90	51	90	126	48 duplicate
6213	55 [612; 4-Aminobutyric acid]	139	[700; Ergosta-5,7-dien-3-ol]	24	0.043	0.194	7.168	0.299	52	89	47	94	6	138 original
6209	55 [612; 4-Aminobutyric acid]	135	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	43	0.025	-0.131	27.189	0.387	53	88	58	83	88	118 original
6210	55 [612; 4-Aminobutyric acid]	138	[748; D-Sedoheptulose-7-phosphate (7TMS)]	11	0.018	0.007	14.337	0.306	54	87	55	86	24	136 original
13286	55 [612; 4-Aminobutyric acid]	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	38	0.010	0.282	15.818	0.530	55	86	44	97	31	58 duplicate
10411	55 [612; 4-Aminobutyric acid]	4	Phosphoric acid	41	-0.005	-0.065	47.705	0.418	56	85	57	84	135	110 duplicate
6214	55 [612; 4-Aminobutyric acid]	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	34	-0.084	0.079	9.717	0.384	57	84	54	87	12	121 original
6168	55 [612; 4-Aminobutyric acid]	94	Hexadecanoic acid	43	-0.087	-0.237	35.811	0.502	58	83	62	79	11	69 original
15356	55 [612; 4-Aminobutyric acid]	47	[NA]	43	-0.101	-0.147	21.220	0.308	59	82	59	82	62	135 duplicate
6183	55 [612; 4-Aminobutyric acid]	109	Octadecanoic acid	43	-0.107	-0.388	36.333	0.516	60	81	73	68	113	65 original
6149	55 [612; 4-Aminobutyric acid]	75	Lysine	43	-0.127	-0.298	52.361	0.584	61	80	66	75	139	25 original
6186	55 [612; 4-Aminobutyric acid]	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	42	-0.143	-0.351	11.228	0.393	62	79	70	71	18	118 original
6190	55 [612; 4-Aminobutyric acid]	116	[882; Pseudouridine (5TMS)]	24	-0.152	-0.043	14.360	0.331	63	78	56	85	25	132 original
6185	55 [612; 4-Aminobutyric acid]	111	[583; Erythritol (4TMS)]	26	-0.169	-0.305	7.935	0.311	64	77	67	74	7	134 original
6204	55 [612; 4-Aminobutyric acid]	130	Trehalose	42	-0.185	-0.149	42.771	0.304	65	76	60	81	123	137 original
6176	55 [612; 4-Aminobutyric acid]	102	[904; Galactose methoxyamine (5TMS)]	43	-0.187	-0.296	18.438	0.335	66	75	65	76	42	131 original
6192	55 [612; 4-Aminobutyric acid]	118	[928; Glucopyranose-6-phosphate (6TMS)]	37	-0.189	-0.554	20.355	0.358	67	74	81	60	53	129 original
6174	55 [612; 4-Aminobutyric acid]	100	[857; Mannitol (6TMS)]	43	-0.192	-0.318	23.743	0.361	68	73	68	73	78	128 original
6170	55 [612; 4-Aminobutyric acid]	96	myo-Inositol	36	-0.203	-0.174	9.778	0.235	69	72	61	80	14	140 original
6138	55 [612; 4-Aminobutyric acid]	64	[789; Tyramine (3TMS)]	42	-0.206	-0.590	20.262	0.419	70	71	85	56	51	109 original
6212	55 [612; 4-Aminobutyric acid]	138	[674; Ergosterol (1TMS)]	29	-0.212	-0.269	10.345	0.414	71	70	63	78	16	112 original
12224	55 [612; 4-Aminobutyric acid]	18	[590; 1-Acetyl-2-thiohydantoin]	43	-0.236	-0.469	23.333	0.380	72	69	78	63	77	123 duplicate
11471	55 [612; 4-Aminobutyric acid]	12	Glyceric acid	42	-0.243	-0.452	14.641	0.404	73	68	76	65	28	115 duplicate
6148	55 [612; 4-Aminobutyric acid]	74	[912; Tetradecanoic acid (1TMS)]	43	-0.262	-0.444	21.572	0.478	74	67	75	68	67	80 original
6157	55 [612; 4-Aminobutyric acid]	83	Sorbitol	43	-0.278	-0.284	36.630	0.495	75	66	64	77	114	73 original
6159	55 [612; 4-Aminobutyric acid]	85	[529; Methylcitric acid (4TMS)]	42	-0.282	-0.374	19.927	0.383	76	65	71	70	47	122 original
6207	55 [612; 4-Aminobutyric acid]	133	[855; Squalene]	43	-0.285	-0.381	23.022	0.375	77	64	72	69	73	125 original
11852	55 [612; 4-Aminobutyric acid]	15	Alanine	43	-0.307	-0.827	34.170	0.613	78	63	113	28	108	10 duplicate
9997	55 [612; 4-Aminobutyric acid]	1	[938; Sulfuric acid (2TMS)]	16	-0.317	-0.697	13.188	0.430	79	62	102	39	22	107 duplicate
6132	55 [612; 4-Aminobutyric acid]	58	[636; 4R-Acetaldo-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	43	-0.318	-0.480	32.562	0.539	80	61	79	62	105	51 original
12587	55 [612; 4-Aminobutyric acid]	21	[678; N,N-D-(2-Hydroxyethyl)-methanamine (2TMS)]	43	-0.333	-0.511	30.331	0.442	81	60	80	61	100	101 duplicate
6153	55 [612; 4-Aminobutyric acid]	79	Glucose	43	-0.340	-0.901	47.115	0.648	82	59	133	8	134	6 original
6200	55 [612; 4-Aminobutyric acid]	126	[559; Erythritol (4TMS)]	24	-0.348	-0.464	18.417	0.559	83	58	77	64	41	40 original
6206	55 [612; 4-Aminobutyric acid]	132	[895; Isomaltose methoxyamine (8TMS)]	23	-0.375	-0.585	14.566	0.280	84	57	83	58	27	139 original

6171	55 [612; 4-Aminobutyric acid 97	756; beta-D-Methylglucopyranoside (4TMS)]	31	-0.381	-0.822	27.809	0.533	85	56	112	29	92	54 original
6179	55 [612; 4-Aminobutyric acid 105	705; 2-Ketoglucuronic acid (5TMS)]	27	-0.385	-0.419	20.352	0.531	86	55	74	67	52	57 original
6165	55 [612; 4-Aminobutyric acid 91	766; beta-D-Methylglucopyranoside (4TMS)]	33	-0.389	-0.581	21.740	0.550	87	54	82	59	68	48 original
6194	55 [612; 4-Aminobutyric acid 120	945; Uridine (3TMS)]	43	-0.398	-0.324	24.905	0.456	88	53	69	72	85	95 original
6201	55 [612; 4-Aminobutyric acid 127	777; Fructose-6-phosphate methoxyamine (6TMS)]	18	-0.399	-0.613	16.469	0.417	89	52	87	54	36	111 original
13511	55 [612; 4-Aminobutyric acid 29	Erythritol	43	-0.404	-0.639	19.582	0.471	90	51	92	49	45	84 duplicate
6202	55 [612; 4-Aminobutyric acid 128	824; D-Sedoheptulose-7-phosphate (7TMS)]	25	-0.413	-0.655	20.113	0.364	91	50	94	47	48	127 original
13172	55 [612; 4-Aminobutyric acid 26	Citramalic acid	43	-0.442	-0.588	30.761	0.436	92	48	84	57	102	105 duplicate
6175	55 [612; 4-Aminobutyric acid 101	832; Dopamine (4TMS)]	43	-0.442	-0.628	21.393	0.588	93	49	90	51	65	24 original
14474	55 [612; 4-Aminobutyric acid 38	708; 2,3-Dimethylsuccinic acid (2TMS)]	43	-0.444	-0.667	22.270	0.448	94	47	96	45	69	100 duplicate
11342	55 [612; 4-Aminobutyric acid 11	Succinic acid	43	-0.453	-0.694	22.746	0.461	95	46	101	40	71	98 duplicate
6187	55 [612; 4-Aminobutyric acid 113	Galactose-6-phosphate	41	-0.456	-0.879	20.526	0.564	96	45	127	14	55	37 original
13399	55 [612; 4-Aminobutyric acid 28	Malic acid	43	-0.464	-0.655	24.299	0.526	97	43	93	48	80	61 duplicate
14777	55 [612; 4-Aminobutyric acid 41	639; Proline (2TMS)]	43	-0.464	-0.710	29.229	0.448	98	44	103	38	98	99 duplicate
6188	55 [612; 4-Aminobutyric acid 114	Fructose-6-phosphate	33	-0.466	-0.875	17.816	0.539	99	42	126	15	39	52 original
6173	55 [612; 4-Aminobutyric acid 99	662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	21	-0.467	-0.671	12.586	0.377	100	41	98	43	20	124 original
15071	55 [612; 4-Aminobutyric acid 44	910; 2-Ketoglucuronic acid methoxyamine (4TMS)]	29	-0.473	-0.638	23.238	0.486	101	40	91	50	76	78 duplicate
10582	55 [612; 4-Aminobutyric acid 6	Glycerol	43	-0.486	-0.872	51.585	0.495	102	39	124	17	138	72 duplicate
6199	55 [612; 4-Aminobutyric acid 125	892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru	43	-0.498	-0.956	42.830	0.534	103	38	140	1	124	53 original
14677	55 [612; 4-Aminobutyric acid 40	680; 2,3-Dimethylsuccinic acid (2TMS)]	43	-0.506	-0.655	45.619	0.519	104	37	95	46	131	64 duplicate
6189	55 [612; 4-Aminobutyric acid 115	Glucose-6-phosphate	41	-0.507	-0.890	37.089	0.497	105	36	130	11	117	70 original
6177	55 [612; 4-Aminobutyric acid 14	Fumaric acid	42	-0.508	-0.667	23.124	0.569	106	35	97	44	74	33 original
11726	55 [612; 4-Aminobutyric acid 103	648; Ethylamine (2TMS)]	43	-0.513	-0.676	16.323	0.461	107	34	100	41	34	85 duplicate
6154	55 [612; 4-Aminobutyric acid 80	772; D-Glucose (5TMS)]	42	-0.519	-0.838	41.827	0.468	108	33	118	23	122	91 original
6178	55 [612; 4-Aminobutyric acid 104	795; Erythritol (4TMS)]	43	-0.524	-0.763	22.816	0.602	109	31	109	32	72	15 original
6161	55 [612; 4-Aminobutyric acid 87	945; beta-D-Glucopyranose (5TMS)]	43	-0.524	-0.888	45.795	0.441	110	32	129	12	132	103 original
6191	55 [612; 4-Aminobutyric acid 117	724; Glycerol (3TMS)]	35	-0.529	-0.624	20.260	0.470	111	30	89	52	50	85 original
12101	55 [612; 4-Aminobutyric acid 17	700; 2-methyl-1,2-propanediol (2TMS)]	43	-0.535	-0.755	30.215	0.505	112	29	107	34	99	68 duplicate
6197	55 [612; 4-Aminobutyric acid 123	945; Galactofuranose-6-phosphate (7TMS)]	43	-0.539	-0.907	27.341	0.592	113	28	134	7	89	22 original
11977	55 [612; 4-Aminobutyric acid 16	644; 2-Methyl-1,3-butanediol (2TMS)]	43	-0.546	-0.763	30.393	0.591	114	26	108	33	101	23 duplicate
12941	55 [612; 4-Aminobutyric acid 24	725; 2-Ketoclanic acid (2TMS)]	43	-0.546	-0.813	13.645	0.596	115	27	111	30	121	17 duplicate
12706	55 [612; 4-Aminobutyric acid 22	690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	34	-0.547	-0.610	13.645	0.405	116	25	86	55	23	114 duplicate
14576	55 [612; 4-Aminobutyric acid 39	829; 1-Phenylethanol (1TMS)]	42	-0.549	-0.715	26.748	0.462	117	24	104	37	87	94 duplicate
14162	55 [612; 4-Aminobutyric acid 35	Pyroglutamic acid	43	-0.561	-0.914	50.945	0.571	118	23	136	5	137	30 duplicate
12346	55 [612; 4-Aminobutyric acid 19	Alanine (BP) (3TMS)	43	-0.566	-0.862	27.813	0.550	119	22	123	18	93	46 duplicate
6147	55 [612; 4-Aminobutyric acid 73	708; Glucose methoxyamine (5TMS)]	42	-0.568	-0.838	20.652	0.540	120	21	117	24	58	50 original
15886	55 [612; 4-Aminobutyric acid 54	[NA]	34	-0.569	-0.837	16.336	0.385	121	20	116	25	35	120 duplicate
6166	55 [612; 4-Aminobutyric acid 92	680; Glyceral-2-phosphate (4TMS)]	33	-0.572	-0.942	21.375	0.411	122	19	139	2	63	113 original
6139	55 [612; 4-Aminobutyric acid 65	646; 3-Deoxyglucitol (5TMS)]	42	-0.577	-0.851	21.425	0.545	123	18	122	19	66	47 original
6144	55 [612; 4-Aminobutyric acid 70	693; 2-Furan-2-hydroxyacetic acid (2TMS)]	41	-0.578	-0.901	32.549	0.541	124	17	132	9	104	49 original
6195	55 [612; 4-Aminobutyric acid 121	657; Erythritol (4TMS)]	34	-0.579	-0.674	15.675	0.475	125	16	99	42	30	81 original
57													
6131	55 [612; 4-Aminobutyric acid	757; 2-Desoxy-pentose-3-ylose dimethoxyamine (2TMS)]	34	-0.586	-0.882	24.127	0.469	126	15	128	13	79	88 original
6196	55 [612; 4-Aminobutyric acid 122	644; Erythritol (4TMS)]	31	-0.587	-0.618	16.283	0.463	127	14	88	53	33	93 original
6150	55 [612; 4-Aminobutyric acid 76	Fructose	43	-0.592	-0.930	37.747	0.592	128	13	138	3	120	20 original
15632	55 [612; 4-Aminobutyric acid 50	746; Ribonic acid-1,4-lactone (3TMS)]	40	-0.600	-0.735	12.146	0.460	129	12	105	36	19	97 duplicate
6152	55 [612; 4-Aminobutyric acid 78	Mannose	42	-0.605	-0.839	20.535	0.494	130	11	119	22	56	74 original
6184	55 [612; 4-Aminobutyric acid 110	715; Erythritol (4TMS)]	33	-0.610	-0.751	20.600	0.553	131	10	106	35	57	44 original
6130	55 [612; 4-Aminobutyric acid 56	829; Oxalic acid (3TMS)]	43	-0.612	-0.894	20.164	0.578	132	9	131	10	49	28 original
6136	55 [612; 4-Aminobutyric acid 62	812; D-Xylofuranose (4TMS)]	43	-0.617	-0.850	28.542	0.496	133	8	121	20	96	71 original
15262	55 [612; 4-Aminobutyric acid 46	Arabinose	43	-0.628	-0.908	27.768	0.554	134	7	135	6	81	43 duplicate

6160	55 [612; 4-Aminobutyric acid]	86 [793; D-Galactono-1,4-lactone (4TMS)]	42 -0.631	-0.924	31,029	0.576	135	6	137	4	103	29 original
	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]											
6203	55 [612; 4-Aminobutyric acid]	86 [793; D-Galactono-1,4-lactone (4TMS)]	38 -0.639	-0.833	21,364	0.560	136	5	114	27	64	39 original
6162	55 [612; 4-Aminobutyric acid]	88 Gluconic acid	43 -0.650	-0.839	24,340	0.617	137	3	120	21	83	9 original
6208	55 [612; 4-Aminobutyric acid]	134 Isomaltose	43 -0.650	-0.874	34,329	0.563	138	4	125	16	109	26 original
11599	55 [612; 4-Aminobutyric acid]	13 Uracil	43 -0.874	-0.801	28,273	0.582	139	2	110	31	95	27 duplicate
6180	55 [612; 4-Aminobutyric acid]	106 [733; Threitol (4TMS)]	41 -0.712	-0.834	24,329	0.819	140	1	115	26	82	7 original
6289	56 [829; Orotic acid (3TMS)]	1757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55 0.884	0.982	7,198	0.699	1	141	5	137	14	10 original
15263	56 [829; Orotic acid (3TMS)]	46 Arabinose	64 0.859	0.992	12,722	0.723	2	140	1	141	43	4 duplicate
16000	56 [829; Orotic acid (3TMS)]	13 Uracil	64 0.859	0.975	15,688	0.703	3	139	7	135	66	7 duplicate
6318	56 [829; Orotic acid (3TMS)]	86 [793; D-Galactono-1,4-lactone (4TMS)]	61 0.849	0.985	17,214	0.711	4	138	4	138	76	5 original
6297	56 [829; Orotic acid (3TMS)]	65 [646; 3-Deoxyglucitol (5TMS)]	63 0.847	0.989	3,737	0.740	5	137	3	139	1	1 original
11978	56 [829; Orotic acid (3TMS)]	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	64 0.844	0.970	18,779	0.703	6	136	9	133	82	8 duplicate
6366	56 [829; Orotic acid (3TMS)]	134 Isomaltose	64 0.840	0.990	23,225	0.727	7	135	2	140	105	3 original
12942	56 [829; Orotic acid (3TMS)]	24 [725; 2-Ketooctanoic acid (2TMS)]	64 0.836	0.981	33,102	0.733	8	134	6	136	123	2 duplicate
6361	56 [829; Orotic acid (3TMS)]	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59 0.811	0.972	3,937	0.673	9	133	8	134	3	20 original
14577	56 [829; Orotic acid (3TMS)]	39 [829; 1-Phenylethanol (1TMS)]	63 0.795	0.957	13,013	0.678	10	132	11	131	45	15 duplicate
15987	56 [829; Orotic acid (3TMS)]	54 [NA]	55 0.785	0.960	6,611	0.638	11	131	10	132	10	37 duplicate
12102	56 [829; Orotic acid (3TMS)]	17 [700; 2-methyl-1,2-propanediol (2TMS)]	64 0.774	0.937	17,985	0.628	12	130	13	129	80	40 duplicate
13512	56 [829; Orotic acid (3TMS)]	29 Erythritol	64 0.768	0.932	8,891	0.641	13	128	15	127	23	35 duplicate
6320	56 [829; Orotic acid (3TMS)]	88 Gluconic acid	64 0.768	0.923	10,378	0.692	14	129	17	125	31	11 original
15633	56 [829; Orotic acid (3TMS)]	50 [746; Ribonic acid-1,4-lactone (3TMS)]	61 0.744	0.930	14,703	0.624	15	127	16	126	60	45 duplicate
6294	56 [829; Orotic acid (3TMS)]	62 [812; D-Xylofuranose (4TMS)]	64 0.732	0.935	16,522	0.655	16	126	14	128	72	28 original
14475	56 [829; Orotic acid (3TMS)]	708; 2,3-Dimethylsuccinic acid (2TMS)]	64 0.722	0.948	9,458	0.682	17	125	12	130	26	14 duplicate
11343	56 [829; Orotic acid (3TMS)]	11 Succinic acid	64 0.695	0.906	10,524	0.627	18	124	21	121	34	41 duplicate
6335	56 [829; Orotic acid (3TMS)]	103 [646; Ethylamine (2TMS)]	63 0.693	0.846	10,480	0.597	19	123	32	110	33	59 original
6331	56 [829; Orotic acid (3TMS)]	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41 0.676	0.914	8,103	0.676	20	122	19	123	19	17 original
6324	56 [829; Orotic acid (3TMS)]	92 [680; Glycerol-2-phosphate (4TMS)]	54 0.667	0.850	4,701	0.804	21	121	31	111	6	56 original
6337	56 [829; Orotic acid (3TMS)]	105 [705; 2-Ketogluconic acid (5TMS)]	48 0.644	0.883	7,078	0.625	22	120	26	116	13	44 original
11727	56 [829; Orotic acid (3TMS)]	14 Fumaric acid	64 0.640	0.908	8,395	0.650	23	119	20	122	21	31 duplicate
6305	56 [829; Orotic acid (3TMS)]	73 [708; Glucose methoxyamine (5TMS)]	57 0.629	0.811	6,309	0.552	24	118	39	103	8	71 original
6308	56 [829; Orotic acid (3TMS)]	76 Fructose	64 0.616	0.921	25,160	0.664	25	117	18	124	110	26 original
13400	56 [829; Orotic acid (3TMS)]	28 Malic acid	64 0.614	0.902	12,232	0.665	26	116	23	119	41	25 duplicate
12707	56 [829; Orotic acid (3TMS)]	22 [690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	52 0.612	0.887	8,160	0.598	27	114	25	117	20	58 duplicate
6328	56 [829; Orotic acid (3TMS)]	97 [756; beta-D-Methylglucopyranoside (4TMS)]	52 0.612	0.837	16,537	0.577	28	115	34	108	73	65 original
11472	56 [829; Orotic acid (3TMS)]	12 Glycetic acid	63 0.611	0.841	9,272	0.611	29	113	33	109	25	53 duplicate
14163	56 [829; Orotic acid (3TMS)]	35 Pyroglutamic acid	64 0.592	0.903	43,366	0.654	30	112	22	120	138	30 duplicate
6338	56 [829; Orotic acid (3TMS)]	106 [733; Threitol (4TMS)]	62 0.576	0.871	8,449	0.685	31	111	28	114	22	12 original
6333	56 [829; Orotic acid (3TMS)]	101 [832; Dopamine (4TMS)]	64 0.572	0.754	9,485	0.542	32	110	45	97	28	75 original
6310	56 [829; Orotic acid (3TMS)]	78 Mannose	62 0.561	0.829	6,278	0.590	33	109	35	107	7	60 original
14678	56 [829; Orotic acid (3TMS)]	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	64 0.551	0.825	37,356	0.621	34	107	37	105	133	47 duplicate
6323	56 [829; Orotic acid (3TMS)]	91 [766; beta-D-Methylglucopyranoside (4TMS)]	64 0.551	0.710	13,810	0.501	35	108	51	91	53	89 original
6302	56 [829; Orotic acid (3TMS)]	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57 0.546	0.661	20,841	0.523	36	106	56	86	94	82 original
6357	56 [829; Orotic acid (3TMS)]	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64 0.542	0.863	32,349	0.642	37	105	29	113	122	33 original
6347	56 [829; Orotic acid (3TMS)]	115 Glucose-6-phosphate	62 0.537	0.890	25,542	0.683	38	104	24	118	111	13 original
6360	56 [829; Orotic acid (3TMS)]	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45 0.535	0.861	3,936	0.645	39	103	30	112	2	32 original
13173	56 [829; Orotic acid (3TMS)]	26 Citramalic acid	64 0.505	0.764	19,853	0.527	40	102	43	89	88	78 duplicate
12588	56 [829; Orotic acid (3TMS)]	21 [678; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	64 0.496	0.745	19,193	0.573	41	101	47	95	83	66 duplicate
9998	56 [829; Orotic acid (3TMS)]	1 [938; Sulfuric acid (2TMS)]	36 0.479	0.670	7,459	0.639	43	99	55	87	16	36 duplicate

6353	56 [828; Orotic acid (3TMS 121 [657; Erythritol (4TMS)]	55	0.457	0.726	11,274	0.602	44	98	49	93	37	57 original
6332	56 [828; Orotic acid (3TMS 100 [657; Mannitol (6TMS)]	64	0.454	0.712	12,238	0.544	45	97	50	92	42	74 original
6349	56 [828; Orotic acid (3TMS 117 [724; Glycerol (3TMS)]	56	0.453	0.757	6,377	0.582	46	98	44	98	9	62 original
6319	56 [828; Orotic acid (3TMS 87 [945; beta-D-Glucopyranose (5TMS)]	62	0.453	0.791	35,990	0.650	47	95	40	102	130	72 original
6354	56 [828; Orotic acid (3TMS 122 [644; Erythritol (4TMS)]	52	0.449	0.827	12,137	0.617	48	94	38	108	40	50 original
6352	56 [828; Orotic acid (3TMS 120 [945; Uridine (3TMS)]	54	0.449	0.341	13,166	0.618	49	93	72	70	46	48 original
6342	56 [828; Orotic acid (3TMS 110 [715; Erythritol (4TMS)]	54	0.448	0.822	7,441	0.673	50	92	38	104	15	19 original
10683	56 [828; Orotic acid (3TMS 8 Glycerol	64	0.438	0.770	44,162	0.565	51	91	42	100	140	68 duplicate
6334	56 [828; Orotic acid (3TMS 102 [904; Galactose methoxamine (5TMS)]	64	0.428	0.646	9,467	0.535	52	90	59	83	27	76 original
6317	56 [828; Orotic acid (3TMS 85 [529; Methylcitric acid (4TMS)]	48	0.408	0.639	9,761	0.432	53	89	60	82	29	125 original
6344	56 [828; Orotic acid (3TMS 112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.402	0.657	14,917	0.527	54	88	58	84	61	79 original
15072	56 [828; Orotic acid (3TMS 44 [910; 2-Ketogluconic acid methoxamine (4TMS)]	50	0.388	0.744	6,628	0.629	55	87	48	94	11	39 duplicate
6359	56 [828; Orotic acid (3TMS 127 [777; Fructose-6-phosphate methoxamine (6TMS)]	39	0.385	0.709	4,649	0.660	56	86	52	90	5	27 original
6367	56 [828; Orotic acid (3TMS 135	64	0.346	0.523	16,444	0.494	57	85	65	77	71	93 original
6364	56 [828; Orotic acid (3TMS 132 [902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	42	0.326	0.875	12,004	0.626	58	84	27	115	39	43 original
6345	56 [828; Orotic acid (3TMS 113 Galactose-6-phosphate	62	0.322	0.780	6,952	0.578	59	83	41	101	12	63 original
12225	56 [828; Orotic acid (3TMS 18 [590; 1-Acetyl-2-thiohydantoin]	64	0.304	0.528	11,877	0.449	60	82	64	78	38	115 duplicate
6336	56 [828; Orotic acid (3TMS 104 [795; Erythritol (4TMS)]	63	0.287	0.510	10,369	0.549	61	81	67	75	32	73 original
6312	56 [828; Orotic acid (3TMS 80 [772; D-Glucose (5TMS)]	62	0.281	0.681	31,714	0.521	62	80	53	89	121	84 original
12347	56 [828; Orotic acid (3TMS 19 Alanine (BP) (3TMS)	64	0.280	0.657	14,005	0.559	63	79	57	85	55	69 duplicate
6308	56 [828; Orotic acid (3TMS 74 [912; Tetradecanoic acid (1TMS)]	64	0.271	0.537	10,235	0.476	64	78	63	79	30	104 original
6358	56 [828; Orotic acid (3TMS 126 [559; Erythritol (4TMS)]	45	0.257	0.546	7,818	0.655	65	77	62	80	18	29 original
6346	56 [828; Orotic acid (3TMS 114 Fructose-6-phosphate	53	0.254	0.749	7,590	0.627	66	76	46	98	17	42 original
6348	56 [828; Orotic acid (3TMS 118 [892; Pseudouridine (5TMS)]	30	0.232	0.289	9,198	0.468	67	75	74	68	24	110 original
14778	56 [828; Orotic acid (3TMS 41 [639; Proline (2TMS)]	64	0.229	0.490	16,852	0.488	68	74	68	74	74	97 duplicate
6355	56 [828; Orotic acid (3TMS 123 [945; Galactofuranose-6-phosphate (7TMS)]	64	0.208	0.515	14,436	0.558	69	73	66	76	59	70 original
6325	56 [828; Orotic acid (3TMS 93 [607; Putrescine (4TMS)]	60	0.199	0.286	14,976	0.444	70	72	75	67	62	117 original
15357	56 [828; Orotic acid (3TMS 47 [NA]	64	0.192	0.241	13,719	0.478	71	71	77	65	50	103 duplicate
6328	56 [828; Orotic acid (3TMS 96 myo-Inositol	49	0.189	0.215	16,328	0.338	72	70	79	63	69	139 original
6316	56 [828; Orotic acid (3TMS 84 Mannitol	62	0.177	0.466	33,597	0.464	73	69	69	73	125	112 original
11853	56 [828; Orotic acid (3TMS 15 Alanine	64	0.158	0.429	21,130	0.671	74	68	70	72	96	21 duplicate
6286	56 [828; Orotic acid (3TMS 64 [789; Tyramine (3TMS)]	63	0.144	0.350	10,625	0.428	75	67	71	71	35	128 original
6315	56 [828; Orotic acid (3TMS 83 Sorbitol	58	0.136	-0.294	26,481	0.362	76	66	92	50	114	138 original
6311	56 [828; Orotic acid (3TMS 79 Glucose	64	0.119	0.621	36,844	0.621	77	65	61	81	131	46 original
6343	56 [828; Orotic acid (3TMS 111 [583; Erythritol (4TMS)]	42	0.089	0.280	19,316	0.423	78	64	76	66	84	130 original
6365	56 [828; Orotic acid (3TMS 133 [855; Squalene]	64	0.036	-0.010	13,641	0.351	79	63	83	59	48	138 original
15900	56 [828; Orotic acid (3TMS 53 Glycerol-2-phosphate	64	0.032	-0.090	12,736	0.365	80	62	85	57	44	135 duplicate
6372	56 [828; Orotic acid (3TMS 140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49	0.029	0.146	13,765	0.467	81	61	81	61	51	106 original
6322	56 [828; Orotic acid (3TMS 90 [910; 9-Z-Hexadecanoic acid (1TMS)]	64	-0.006	-0.101	13,662	0.442	82	60	86	56	49	118 original
6341	56 [828; Orotic acid (3TMS 109 Octadecanoic acid	64	-0.008	0.204	24,740	0.489	83	59	73	69	108	95 original
6350	56 [828; Orotic acid (3TMS 118 [928; Glucopyranose-6-phosphate (6TMS)]	58	-0.021	0.241	11,097	0.467	84	58	78	64	36	108 original
6326	56 [828; Orotic acid (3TMS 94 Hexadecanoic acid	64	-0.053	0.196	24,942	0.483	85	57	80	62	109	89 original
6371	56 [828; Orotic acid (3TMS 139 [700; Ergosta-5,7-dien-3-ol]	38	-0.055	-0.159	16,899	0.467	86	56	88	54	75	107 original
6295	56 [828; Orotic acid (3TMS 63 Glutamine	52	-0.074	-0.763	23,621	0.705	87	55	123	19	107	6 original
6373	56 [828; Orotic acid (3TMS 141 Lanosta-8,24-dien-3-beta-ol	61	-0.080	-0.033	14,232	0.481	88	54	84	58	57	100 original
6304	56 [828; Orotic acid (3TMS 72 [919; D-Xylopyranose (4TMS)]	63	-0.123	-0.153	14,136	0.360	89	53	87	55	56	137 original
6370	56 [828; Orotic acid (3TMS 138 [674; Ergosterol (1TMS)]	46	-0.134	-0.007	15,770	0.471	90	52	82	60	68	105 original
6339	56 [828; Orotic acid (3TMS 107 9-Z-Octadecanoic acid	64	-0.157	-0.352	19,819	0.435	91	51	94	48	87	122 original
6351	56 [828; Orotic acid (3TMS 119 [931; myo-Inositol-2-phosphate (7TMS)]	64	-0.169	-0.251	15,074	0.514	92	50	90	52	64	86 original
6369	56 [828; Orotic acid (3TMS 137 Ergosterol	64	-0.176	-0.235	20,185	0.467	93	48	89	53	92	109 original



6303	56 [828; Orotic acid (3TMS)	71	[731; Erythrose (3TMS)]	64	-0.176	-0.272	17.316	0.442	94	49	91	51	77	120 original
14975	56 [828; Orotic acid (3TMS)	43	[548; Leucine (2TBS)]	60	-0.176	-0.363	15.020	0.489	95	47	95	47	63	98 duplicate
10412	56 [828; Orotic acid (3TMS)	4	Phosphoric acid	51	-0.198	-0.413	38.389	0.301	96	46	98	44	138	141 duplicate
15812	56 [828; Orotic acid (3TMS)	52	[NA]	48	-0.210	-0.681	23.067	0.673	97	45	116	28	102	18 duplicate
6356	56 [828; Orotic acid (3TMS)	124	[734; 1-Monoolcylglycerol (2TMS); 1-Monohexadecylglycerol (1TMS)]	59	-0.251	-0.401	22.229	0.424	98	44	97	45	101	129 original
6290	56 [828; Orotic acid (3TMS)	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	-0.251	-0.381	21.895	0.394	99	43	98	46	99	133 original
6362	56 [828; Orotic acid (3TMS)	130	Trehalose	63	-0.262	-0.341	33.451	0.374	100	42	93	49	124	134 original
6293	56 [828; Orotic acid (3TMS)	61	[NA]	17	-0.270	-0.494	13.804	0.499	101	41	100	42	52	90 original
6368	56 [828; Orotic acid (3TMS)	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	64	-0.284	-0.478	4.514	0.494	102	40	99	43	4	94 original
6300	56 [828; Orotic acid (3TMS)	68	[570; Hypoxanthine (2TMS)]	20	-0.295	-0.928	13.986	0.621	103	39	138	4	54	48 original
13058	56 [828; Orotic acid (3TMS)	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.303	-0.895	20.558	0.641	104	38	135	7	93	34 duplicate
6330	56 [828; Orotic acid (3TMS)	98	[697; Ribose-5-phosphate methoxymine (5TMS)]	48	-0.319	-0.759	20.056	0.523	105	37	122	20	89	81 original
6307	56 [828; Orotic acid (3TMS)	75	Lysine	64	-0.325	-0.506	43.652	0.448	106	36	101	41	139	116 original
10817	56 [828; Orotic acid (3TMS)	7	Threonine	64	-0.336	-0.532	34.247	0.418	107	34	102	40	127	131 duplicate
6340	56 [828; Orotic acid (3TMS)	108	Octadecenoic acid	64	-0.336	-0.537	14.240	0.400	108	35	103	39	58	132 original
13287	56 [828; Orotic acid (3TMS)	27	[815; (E)-4-Methyl-5-hydroxy-3-pentan-2-one (1TMS)]	53	-0.340	-0.780	23.163	0.566	109	33	124	18	103	67 duplicate
15168	56 [828; Orotic acid (3TMS)	45	Homocysteine	61	-0.357	-0.571	21.050	0.429	110	32	105	37	95	126 duplicate
6321	56 [828; Orotic acid (3TMS)	89	[775; Dopamine (4TMS)]	35	-0.365	-0.869	22.089	0.614	111	31	133	9	100	51 original
12825	56 [828; Orotic acid (3TMS)	23	Homoserine	64	-0.368	-0.814	20.159	0.610	112	30	127	15	90	54 duplicate
10137	56 [828; Orotic acid (3TMS)	2	Serine	62	-0.400	-0.608	26.707	0.435	113	29	109	33	117	121 duplicate
15542	56 [828; Orotic acid (3TMS)	49	[877; Pyrophosphoric acid (4TMS)]	64	-0.410	-0.593	33.224	0.458	114	28	107	35	104	114 duplicate
14268	56 [828; Orotic acid (3TMS)	36	[596; N-Acetylglutamic acid (2TMS)]	64	-0.424	-0.597	33.607	0.428	115	27	108	34	126	127 duplicate
6298	56 [828; Orotic acid (3TMS)	66	Glycine acid-3-phosphate	64	-0.429	-0.628	13.552	0.464	116	26	110	32	47	111 original
14057	56 [828; Orotic acid (3TMS)	34	Aspartic acid	64	-0.438	-0.589	37.579	0.512	117	25	108	38	135	87 duplicate
10950	56 [828; Orotic acid (3TMS)	8	Isoleucine	55	-0.448	-0.566	26.237	0.338	118	24	104	38	113	140 duplicate
13733	56 [828; Orotic acid (3TMS)	31	[822; Parabenic acid (2TMS)]	64	-0.462	-0.709	15.712	0.535	119	23	119	23	67	77 duplicate
6327	56 [828; Orotic acid (3TMS)	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	-0.473	-0.708	19.658	0.523	120	22	118	24	86	83 original
6292	56 [828; Orotic acid (3TMS)	60	Glycerol-3-phosphate	64	-0.474	-0.651	26.538	0.519	121	21	112	30	116	85 original
11082	56 [828; Orotic acid (3TMS)	9	Proline	63	-0.482	-0.649	34.684	0.433	122	20	111	31	128	124 duplicate
13950	56 [828; Orotic acid (3TMS)	33	Methionine	64	-0.486	-0.675	19.543	0.526	123	19	115	27	85	80 duplicate
14372	56 [828; Orotic acid (3TMS)	37	Phenylalanine	64	-0.489	-0.719	27.448	0.485	124	18	121	21	118	98 duplicate
6299	56 [828; Orotic acid (3TMS)	67	Citric acid	64	-0.492	-0.674	28.106	0.460	125	17	114	28	119	113 original
6363	56 [828; Orotic acid (3TMS)	131	[626; 5-Methylthioadenosine (3TMS)]	55	-0.502	-0.713	17.451	0.594	126	16	120	22	78	61 original
15450	56 [828; Orotic acid (3TMS)	48	Asparagine	64	-0.508	-0.862	21.425	0.667	127	15	131	11	97	24 duplicate
13623	56 [828; Orotic acid (3TMS)	30	[915; Ethyl-3(2H)-thiophenone]	64	-0.528	-0.673	35.742	0.442	128	14	113	29	129	119 duplicate
15723	56 [828; Orotic acid (3TMS)	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.556	-0.816	18.555	0.481	129	13	128	14	81	101 duplicate
13942	56 [828; Orotic acid (3TMS)	32	[729; N,N-Dimethyllysine methyl ester]	63	-0.585	-0.821	23.462	0.608	130	12	129	13	106	55 duplicate
6291	56 [828; Orotic acid (3TMS)	59	Ornithine; Arginine	64	-0.591	-0.702	45.191	0.506	131	11	117	25	141	88 original
10548	56 [828; Orotic acid (3TMS)	5	Leucine	45	-0.602	-0.792	16.364	0.499	132	10	125	17	70	91 duplicate
16073	56 [828; Orotic acid (3TMS)	55	[612; 4-Aminobutyric acid (2TBS)]	43	-0.612	-0.894	20.164	0.578	133	9	134	8	91	64 duplicate
10275	56 [828; Orotic acid (3TMS)	3	Ethanolamine	62	-0.622	-0.866	17.553	0.611	134	8	132	10	79	52 duplicate
12468	56 [828; Orotic acid (3TMS)	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.639	-0.960	15.442	0.668	135	7	140	2	65	23 duplicate
6301	56 [828; Orotic acid (3TMS)	69	Arginine	60	-0.643	-0.899	29.489	0.634	136	6	136	6	120	38 original
6309	56 [828; Orotic acid (3TMS)	77	[926; beta-[[[5-methyl-2-thienyl]methyl]eneamino-benzeneacetic acid methyl ester]	62	-0.669	-0.824	36.863	0.480	137	5	130	12	132	102 original
11213	56 [828; Orotic acid (3TMS)	10	Glycine	64	-0.681	-0.956	26.528	0.701	138	4	139	3	115	9 duplicate
14877	56 [828; Orotic acid (3TMS)	42	Glutamic acid	60	-0.694	-0.810	37.440	0.498	139	3	126	16	134	82 duplicate
6314	56 [828; Orotic acid (3TMS)	82	Lysine	39	-0.706	-0.971	26.008	0.678	140	2	141	1	112	16 original

6313	56 [829; Orotic acid (3TMS)	81 Tyrosine		64 -0.709	-0.916	40.253	0.668	141	1	137	5	137	22 original
6381	57 [757; 2-Desoxy-pentose<	65 [646; 3-Deoxyglucitol (5TMS)]		55 0.922	0.977	5.371	0.712	1	141	5	137	2	3 original
12684	57 [757; 2-Desoxy-pentose<	46 Arabinose		55 0.887	0.991	7.306	0.714	2	140	1	141	6	2 duplicate
16232	57 [757; 2-Desoxy-pentose<	58 [828; Orotic acid (3TMS)]		55 0.884	0.982	7.198	0.699	3	139	4	138	5	5 duplicate
12943	57 [757; 2-Desoxy-pentose<	24 [725; 2-Ketocacetic acid (2TMS)]		55 0.879	0.962	25.715	0.702	4	138	7	135	114	4 duplicate
6450	57 [757; 2-Desoxy-pentose<	134 Isomaltose		55 0.868	0.983	17.015	0.718	5	138	3	139	68	1 original
11979	57 [757; 2-Desoxy-pentose<	16 [644; 2-Methyl-1,3-butanediol (2TMS)]		55 0.868	0.944	13.530	0.662	6	137	9	133	44	17 duplicate
11601	57 [757; 2-Desoxy-pentose<	13 Uracil		55 0.867	0.959	10.545	0.662	7	135	8	134	20	18 duplicate
6402	57 [757; 2-Desoxy-pentose<	86 [793; D-Galactono-1,4-lactone (4TMS)]		52 0.845	0.988	11.628	0.687	8	134	2	140	27	7 original
		129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-											
6445	57 [757; 2-Desoxy-pentose<	[Glc]		54 0.831	0.964	5.055	0.663	9	133	6	136	1	15 original
15634	57 [757; 2-Desoxy-pentose<	50 [746; Ribonic acid-1,4-lactone (3TMS)]		55 0.815	0.929	21.073	0.597	10	132	13	129	89	46 duplicate
121203	57 [757; 2-Desoxy-pentose<	17 [700; 2-methyl-1,2-propanediol (2TMS)]		55 0.779	0.910	13.138	0.603	11	131	14	128	40	43 duplicate
13513	57 [757; 2-Desoxy-pentose<	29 Erythritol		55 0.774	0.896	12.219	0.634	12	130	18	124	30	29 duplicate
6404	57 [757; 2-Desoxy-pentose<	88 Gluconic acid		55 0.768	0.889	8.043	0.659	13	129	20	122	8	19 original
15988	57 [757; 2-Desoxy-pentose<	54 [NA]		51 0.765	0.932	12.553	0.662	14	128	12	130	33	16 duplicate
146578	57 [757; 2-Desoxy-pentose<	39 [829; 1-Phenylethanol (1TMS)]		55 0.762	0.933	8.133	0.651	15	127	11	131	11	21 duplicate
63478	57 [757; 2-Desoxy-pentose<	62 [812; D-Xylofuranose (4TMS)]		55 0.720	0.941	12.761	0.669	16	126	10	132	36	10 original
44476	57 [757; 2-Desoxy-pentose<	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]		55 0.708	0.908	10.152	0.641	17	125	15	127	16	26 duplicate
11344	57 [757; 2-Desoxy-pentose<	11 Succinic acid		55 0.702	0.891	10.985	0.617	18	124	19	123	22	38 duplicate
6415	57 [757; 2-Desoxy-pentose<	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]		38 0.698	0.853	13.913	0.664	19	123	27	115	48	13 original
6408	57 [757; 2-Desoxy-pentose<	92 [680; Glycerol-2-phosphate (4TMS)]		51 0.680	0.872	8.413	0.617	20	122	23	119	12	39 original
6421	57 [757; 2-Desoxy-pentose<	105 [705; 2-Ketoglucuronic acid (5TMS)]		48 0.649	0.884	6.395	0.631	21	121	21	121	4	32 original
111728	57 [757; 2-Desoxy-pentose<	14 Fumaric acid		55 0.634	0.802	14.285	0.646	22	119	17	125	51	24 duplicate
11473	57 [757; 2-Desoxy-pentose<	12 Glycic acid		55 0.626	0.807	15.811	0.623	23	120	33	109	61	35 duplicate
6419	57 [757; 2-Desoxy-pentose<	103 [648; Ethylamine (2TMS)]		47 0.600	0.845	14.116	0.628	25	118	37	105	13	74 original
12708	57 [757; 2-Desoxy-pentose<	22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]		55 0.600	0.817	11.373	0.591	26	116	32	110	24	34 duplicate
6413	57 [757; 2-Desoxy-pentose<	97 [756; beta-D-Methylglucopyranoside (4TMS)]		35 0.570	0.560	12.242	0.629	27	115	59	83	31	48 original
9989	57 [757; 2-Desoxy-pentose<	1 [938; Sulfuric acid (2TMS)]		55 0.561	0.871	11.201	0.593	28	114	24	118	23	33 duplicate
13401	57 [757; 2-Desoxy-pentose<	28 Malic acid		39 0.541	0.668	9.897	0.420	29	113	51	91	15	47 duplicate
6401	57 [757; 2-Desoxy-pentose<	85 [529; Methylcitric acid (4TMS)]		48 0.539	0.725	9.471	0.488	30	112	41	101	14	79 original
6389	57 [757; 2-Desoxy-pentose<	73 [708; Glucose methoxyamine (5TMS)]		44 0.514	0.829	6.151	0.647	31	111	30	112	3	23 original
6444	57 [757; 2-Desoxy-pentose<	128 [824; D-Scetioheptulose-7-phosphate (7TMS)]		55 0.502	0.907	19.444	0.632	33	109	16	126	80	60 original
6386	57 [757; 2-Desoxy-pentose<	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]		48 0.500	0.582	16.055	0.525	34	108	57	85	64	38 original
14678	57 [757; 2-Desoxy-pentose<	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]		55 0.494	0.770	29.020	0.574	35	107	38	104	129	53 duplicate
6417	57 [757; 2-Desoxy-pentose<	101 [832; Dopamine (4TMS)]		55 0.487	0.649	10.406	0.460	36	106	53	89	19	87 original
6394	57 [757; 2-Desoxy-pentose<	78 Mannose		53 0.478	0.801	10.338	0.568	37	105	34	108	18	58 original
6407	57 [757; 2-Desoxy-pentose<	91 [766; beta-D-Methylglucopyranoside (4TMS)]		55 0.471	0.630	12.787	0.400	38	104	54	88	37	122 original
2589	57 [757; 2-Desoxy-pentose<	21 [672; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]		55 0.463	0.692	14.571	0.558	39	103	45	97	53	61 duplicate
6441	57 [757; 2-Desoxy-pentose<	125 [898; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]		55 0.452	0.828	26.203	0.604	40	102	29	113	118	42 original
6422	57 [757; 2-Desoxy-pentose<	106 [733; Threitol (4TMS)]		53 0.451	0.827	8.100	0.644	41	101	31	111	10	25 original
6436	57 [757; 2-Desoxy-pentose<	120 [945; Uridine (3TMS)]		51 0.451	0.320	12.840	0.609	42	100	72	70	38	41 original
14164	57 [757; 2-Desoxy-pentose<	35 Pyroglutamic acid		55 0.425	0.877	35.051	0.599	43	99	22	120	139	44 duplicate
6431	57 [757; 2-Desoxy-pentose<	115 Glucose-6-phosphate		54 0.423	0.859	19.797	0.664	44	98	26	116	84	12 original
13174	57 [757; 2-Desoxy-pentose<	26 Citramalic acid		55 0.411	0.692	15.313	0.522	45	97	47	95	58	70 duplicate
6418	57 [757; 2-Desoxy-pentose<	102 [904; Galactose methoxyamine (5TMS)]		55 0.393	0.608	13.788	0.510	46	96	55	87	46	73 original
6416	57 [757; 2-Desoxy-pentose<	100 [857; Mannitol (6TMS)]		55 0.389	0.673	11.669	0.543	47	95	50	92	28	63 original
6428	57 [757; 2-Desoxy-pentose<	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (8TMS)]		54 0.374	0.568	21.691	0.494	48	94	58	84	96	76 original
6403	57 [757; 2-Desoxy-pentose<	87 [945; beta-D-Glucopyranose (5TMS)]		53 0.366	0.751	28.723	0.572	49	93	39	103	132	56 original
6426	57 [757; 2-Desoxy-pentose<	110 [715; Erythritol (4TMS)]		51 0.360	0.799	11.421	0.680	50	92	35	107	25	9 original

6433	57 [757; 2-Desoxy-pentose-117 [724; Glyceral (3TMS)]	51	0.358	0.708	10,789	0.569	51	91	44	98	21	57 original
6437	57 [757; 2-Desoxy-pentose-121 [657; Erythritol (4TMS)]	49	0.349	0.654	17,272	0.584	52	90	52	90	69	50 original
6438	57 [757; 2-Desoxy-pentose-122 [644; Erythritol (4TMS)]	49	0.342	0.791	17,343	0.635	53	89	36	106	70	28 original
6443	57 [757; 2-Desoxy-pentose-127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.336	0.691	10,241	0.649	54	88	48	94	17	22 original
6409	57 [757; 2-Desoxy-pentose-93 [607; Putrescine (4TMS)]	53	0.334	0.300	21,065	0.357	55	87	74	68	88	133 original
6400	57 [757; 2-Desoxy-pentose-84 Mannitol	53	0.325	0.468	25,707	0.460	56	86	63	79	113	88 original
6448	57 [757; 2-Desoxy-pentose-132 [895; Isomaltose methoxyamine (8TMS)]	41	0.324	0.870	16,629	0.817	57	85	25	117	65	37 original
6451	57 [757; 2-Desoxy-pentose-135 [902; Maltotriose (8TMS); alpha-D-Gal-(1,8)-D-Glc (8TMS)]	55	0.320	0.465	13,737	0.457	58	84	64	78	45	90 original
6379	57 [757; 2-Desoxy-pentose-63 Glutamine	43	0.311	-0.666	25,827	0.666	59	83	119	23	115	11 original
15073	57 [757; 2-Desoxy-pentose-44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	49	0.310	0.727	8,051	0.639	60	82	40	102	9	27 duplicate
6432	57 [757; 2-Desoxy-pentose-116 [882; Pseudouridine (5TMS)]	26	0.268	0.313	11,560	0.407	61	81	73	69	26	117 original
10694	57 [757; 2-Desoxy-pentose-6 Glyceral	55	0.259	0.692	35,599	0.560	62	80	46	98	140	60 duplicate
6390	57 [757; 2-Desoxy-pentose-74 [912; Tetradecanoic acid (1TMS)]	55	0.251	0.511	13,140	0.433	63	79	62	80	41	105 original
6406	57 [757; 2-Desoxy-pentose-90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	55	0.223	0.158	13,890	0.407	64	78	82	60	47	118 original
6442	57 [757; 2-Desoxy-pentose-126 [559; Erythritol (4TMS)]	45	0.212	0.558	12,985	0.654	65	77	60	82	39	20 original
15358	57 [757; 2-Desoxy-pentose-47 [NA]	55	0.195	0.173	15,346	0.458	66	76	79	63	59	89 duplicate
12226	57 [757; 2-Desoxy-pentose-18 [590; 1-Acetyl-2-thiohydantoin]	55	0.193	0.419	12,659	0.437	67	75	66	76	35	101 duplicate
15901	57 [757; 2-Desoxy-pentose-53 Glyceral-2-phosphate	55	0.169	-0.008	18,383	0.387	68	74	88	56	77	129 duplicate
6429	57 [757; 2-Desoxy-pentose-113 Galactose-6-phosphate	54	0.157	0.713	12,118	0.572	69	73	43	99	29	55 original
6396	57 [757; 2-Desoxy-pentose-80 [772; D-Glucose (5TMS)]	53	0.125	0.597	26,016	0.549	70	72	56	86	117	62 original
6456	57 [757; 2-Desoxy-pentose-140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	40	0.108	0.321	19,507	0.434	71	71	71	71	81	104 original
6412	57 [757; 2-Desoxy-pentose-96 myo-Inositol	40	0.105	0.169	21,817	0.251	72	70	80	62	98	141 original
6420	57 [757; 2-Desoxy-pentose-104 [795; Erythritol (4TMS)]	54	0.092	0.419	12,657	0.519	73	69	67	75	34	71 original
15813	57 [757; 2-Desoxy-pentose-52 [NA]	37	0.078	-0.582	27,597	0.574	74	68	108	34	124	54 duplicate
6430	57 [757; 2-Desoxy-pentose-114 Fructose-6-phosphate	47	0.073	0.680	13,377	0.567	75	67	49	93	43	59 original
12348	57 [757; 2-Desoxy-pentose-19 Alanine (BP) (3TMS)	55	0.067	0.554	12,285	0.531	76	66	61	81	32	68 duplicate
6423	57 [757; 2-Desoxy-pentose-107 9-(Z)-Octadecenoic acid	55	0.056	-0.097	15,309	0.432	77	65	90	52	57	106 original
6457	57 [757; 2-Desoxy-pentose-141 Lanosta-8,24-dien-3-beta-ol	52	0.050	0.166	19,514	0.468	78	64	81	61	82	88 original
6399	57 [757; 2-Desoxy-pentose-83 Sorbitol	49	0.046	-0.304	21,708	0.303	79	63	95	47	97	138 original
6427	57 [757; 2-Desoxy-pentose-111 [583; Erythritol (4TMS)]	38	0.041	0.330	25,196	0.435	80	62	70	72	110	103 original
6425	57 [757; 2-Desoxy-pentose-109 Octadecanoic acid	55	0.038	0.300	19,572	0.432	81	61	75	67	83	107 original
6435	57 [757; 2-Desoxy-pentose-119 [931; myo-Inositol-2-phosphate (7TMS)]	55	0.033	-0.034	15,203	0.499	82	60	87	55	56	75 original
14778	57 [757; 2-Desoxy-pentose-41 [639; Proline (2TMS)]	55	0.017	0.359	14,114	0.477	83	59	69	73	49	83 duplicate
6449	57 [757; 2-Desoxy-pentose-133 [855; Squalene]	55	0.005	0.032	15,040	0.470	84	58	85	57	55	136 original
6410	57 [757; 2-Desoxy-pentose-94 Hexadecanoic acid	55	-0.018	0.245	18,814	0.470	85	57	76	68	78	84 original
6439	57 [757; 2-Desoxy-pentose-123 [945; Galactofuranose-6-phosphate (7TMS)]	55	-0.026	0.369	13,182	0.528	86	56	68	74	42	67 original
6455	57 [757; 2-Desoxy-pentose-139 [700; Ergosta-5,7-dien-3-ol]	30	-0.039	-0.064	22,419	0.441	87	55	88	54	101	98 original
6453	57 [757; 2-Desoxy-pentose-137 Ergosterol	55	-0.040	-0.089	17,076	0.431	88	54	89	53	67	109 original
6388	57 [757; 2-Desoxy-pentose-72 [919; D-Xylopyranose (4TMS)]	54	-0.072	-0.139	17,591	0.355	89	53	91	51	75	134 original
6380	57 [757; 2-Desoxy-pentose-64 [769; Tyramine (3TMS)]	55	-0.108	0.206	14,325	0.436	90	52	78	64	52	102 original
6377	57 [757; 2-Desoxy-pentose-61 [NA]	55	-0.115	-0.394	15,778	0.455	91	51	98	44	60	92 original
6440	57 [757; 2-Desoxy-pentose-124 [734; 1-Monocleoylglycerol (2TMS); 1-Monohexadecenoylethanol (1TMS)]	50	-0.123	-0.160	28,587	0.413	92	50	92	50	126	115 original
11854	57 [757; 2-Desoxy-pentose-15 Alanine	55	-0.126	0.223	17,517	0.680	93	49	77	65	73	8 duplicate
6434	57 [757; 2-Desoxy-pentose-118 [928; Glucopyranose-6-phosphate (6TMS)]	54	-0.126	0.127	15,873	0.432	94	48	83	59	62	108 original
14976	57 [757; 2-Desoxy-pentose-43 [548; Leucine (2TBS)]	51	-0.176	-0.379	15,961	0.399	95	47	96	46	63	123 duplicate
6395	57 [757; 2-Desoxy-pentose-78 Glucose	55	-0.185	0.456	30,205	0.616	96	46	65	77	135	40 original
6424	57 [757; 2-Desoxy-pentose-108 Octadecenoic acid	55	-0.191	-0.395	17,545	0.402	97	45	99	43	74	121 original
6387	57 [757; 2-Desoxy-pentose-71 [731; Erythrose (3TMS)]	55	-0.213	-0.298	15,005	0.404	98	44	94	48	54	120 original
6454	57 [757; 2-Desoxy-pentose-138 [674; Ergosterol (1TMS)]	38	-0.215	0.040	21,565	0.417	99	43	84	58	84	113 original

6452	57 [757; 2-Desoxy-pentose-3]	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.235	-0.458	7.587	0.480	100	42	101	41	7	81 original
13059	57 [757; 2-Desoxy-pentose-3]	25	[709; 2,5-Diaminovalerolactam (2TMS)]	47	-0.241	-0.880	25.233	0.664	101	41	135	7	111	14 duplicate
6405	57 [757; 2-Desoxy-pentose-3]	89	[775; Dopamine (4TMS)]	26	-0.274	-0.843	23.588	0.445	102	40	133	9	105	96 original
15543	57 [757; 2-Desoxy-pentose-3]	49	[877; Pyrophosphoric acid (4TMS)]	55	-0.280	-0.541	28.889	0.442	103	39	105	37	128	97 duplicate
6446	57 [757; 2-Desoxy-pentose-3]	130	Trehalose	55	-0.309	-0.276	25.969	0.416	104	38	93	49	116	114 original
10413	57 [757; 2-Desoxy-pentose-3]	4	Phosphoric acid	42	-0.310	-0.381	30.127	0.273	105	37	97	45	134	139 duplicate
6414	57 [757; 2-Desoxy-pentose-3]	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	40	-0.346	-0.719	25.244	0.453	106	38	123	19	112	93 original
15189	57 [757; 2-Desoxy-pentose-3]	45	Homocysteine	52	-0.354	-0.561	27.551	0.407	107	35	107	35	123	119 duplicate
12626	57 [757; 2-Desoxy-pentose-3]	23	Homoserine	55	-0.362	-0.771	21.263	0.582	108	34	127	15	91	51 duplicate
6447	57 [757; 2-Desoxy-pentose-3]	131	[626; 5-Methylthioadenosine (3TMS)]	47	-0.369	-0.617	23.118	0.524	109	33	113	29	104	69 original
6411	57 [757; 2-Desoxy-pentose-3]	95	[770; 3,4,6-Trisubstitutedphenylmethanolamine (5TMS)]	41	-0.378	-0.632	24.779	0.392	110	32	115	27	108	125 original
6374	57 [757; 2-Desoxy-pentose-3]	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexene (1TMS)]	55	-0.418	-0.408	19.120	0.364	111	31	100	42	79	130 original
6391	57 [757; 2-Desoxy-pentose-3]	75	Lysine	55	-0.429	-0.461	34.462	0.427	112	30	102	40	138	110 original
6393	57 [757; 2-Desoxy-pentose-3]	67	Citric acid	55	-0.430	-0.607	21.398	0.370	113	29	111	31	92	128 original
10818	57 [757; 2-Desoxy-pentose-3]	7	Threonine	55	-0.436	-0.524	26.535	0.342	114	28	104	38	120	135 duplicate
15451	57 [757; 2-Desoxy-pentose-3]	48	Asparagine	55	-0.441	-0.825	21.980	0.631	115	27	131	11	100	31 duplicate
13288	57 [757; 2-Desoxy-pentose-3]	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	44	-0.461	-0.768	27.283	0.514	116	26	126	16	121	72 duplicate
6394	57 [757; 2-Desoxy-pentose-3]	68	[570; Hypoxanthine (2TMS)]	14	-0.473	-0.917	17.186	0.309	117	25	138	4	68	137 original
14269	57 [757; 2-Desoxy-pentose-3]	36	[598; N-Acetylglutamic acid (2TMS)]	55	-0.481	-0.557	26.527	0.393	118	23	106	38	119	124 duplicate
6376	57 [757; 2-Desoxy-pentose-3]	60	Glycerol-3-phosphate	55	-0.481	-0.605	20.600	0.478	119	24	110	32	85	82 original
14058	57 [757; 2-Desoxy-pentose-3]	34	Aspartic acid	55	-0.494	-0.609	29.811	0.445	120	22	112	30	133	95 duplicate
14373	57 [757; 2-Desoxy-pentose-3]	37	Phenylalanine	55	-0.502	-0.693	21.165	0.446	121	21	122	20	90	94 duplicate
13951	57 [757; 2-Desoxy-pentose-3]	33	Methionine	55	-0.506	-0.650	20.842	0.455	122	20	116	28	87	91 duplicate
10951	57 [757; 2-Desoxy-pentose-3]	8	Isoleucine	46	-0.509	-0.515	23.024	0.268	123	19	103	39	103	140 duplicate
13734	57 [757; 2-Desoxy-pentose-3]	31	[622; Parabenic acid (2TMS)]	53	-0.514	-0.688	20.820	0.533	124	18	121	21	86	65 duplicate
10138	57 [757; 2-Desoxy-pentose-3]	2	Serine	55	-0.528	-0.583	24.510	0.362	125	17	109	33	107	131 duplicate
6382	57 [757; 2-Desoxy-pentose-3]	66	Glyceric acid-3-phosphate	55	-0.546	-0.658	17.446	0.481	126	16	117	25	71	80 original
11083	57 [757; 2-Desoxy-pentose-3]	9	Proline	54	-0.563	-0.622	29.399	0.362	127	15	114	28	130	132 duplicate
13624	57 [757; 2-Desoxy-pentose-3]	30	[815; Ethyl-3-(2H)-thiophenone]	55	-0.568	-0.661	28.709	0.373	128	14	118	24	127	127 duplicate
15724	57 [757; 2-Desoxy-pentose-3]	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	35	-0.580	-0.773	22.924	0.385	129	13	128	14	102	126 duplicate
16074	57 [757; 2-Desoxy-pentose-3]	55	[612; 4-Aminobutyric acid (2TBS)]	34	-0.588	-0.882	24.127	0.469	130	12	136	6	106	85 duplicate
10276	57 [757; 2-Desoxy-pentose-3]	3	Ethanolamine	53	-0.621	-0.830	21.849	0.534	131	11	132	10	99	64 duplicate
6375	57 [757; 2-Desoxy-pentose-3]	59	Ornithine; Arginine	55	-0.624	-0.678	35.713	0.437	132	10	120	22	141	100 original
10549	57 [757; 2-Desoxy-pentose-3]	5	Leucine	36	-0.638	-0.746	17.887	0.439	133	9	124	18	76	99 duplicate
6385	57 [757; 2-Desoxy-pentose-3]	69	Arginine	51	-0.641	-0.879	25.052	0.598	134	8	134	8	109	45 original
6393	57 [757; 2-Desoxy-pentose-3]	8	[826; beta-[[[5-methyl-2-thienyl]methyl]amino]benzoic acid methyl ester]	53	-0.656	-0.787	29.457	0.409	135	7	129	13	131	116 original
13843	57 [757; 2-Desoxy-pentose-3]	32	[729; N,N-Dimethyllysine methyl ester]	54	-0.677	-0.801	27.532	0.575	136	6	130	12	122	52 duplicate
11214	57 [757; 2-Desoxy-pentose-3]	10	Glycine	55	-0.694	-0.944	21.636	0.687	137	5	139	3	95	6 duplicate
14878	57 [757; 2-Desoxy-pentose-3]	42	Glutamic acid	51	-0.700	-0.764	30.889	0.419	138	4	125	17	136	112 duplicate
6398	57 [757; 2-Desoxy-pentose-3]	82	Lysine	30	-0.715	-0.949	21.457	0.568	139	3	140	2	93	49 original
12469	57 [757; 2-Desoxy-pentose-3]	20	[619; 2,3,4'-Bishydroxyphenyl-2-oxoethylamine (4TMS)]	22	-0.723	-0.955	17.475	0.494	140	2	141	1	72	77 duplicate
6397	57 [757; 2-Desoxy-pentose-3]	81	Tyrosine	55	-0.731	-0.894	31.287	0.621	141	1	137	5	137	36 original
6474	58 [636; 4R-Acetamido-2,3	75	Lysine	64	0.755	0.920	25.701	0.541	1	141	1	141	122	7 original
10139	58 [636; 4R-Acetamido-2,3	2	Serine	62	0.537	0.827	9.857	0.532	2	140	3	139	13	10 duplicate
11084	58 [636; 4R-Acetamido-2,3	9	Proline	63	0.479	0.788	14.123	0.501	3	139	4	138	41	18 duplicate
13289	58 [636; 4R-Acetamido-2,3	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	0.470	0.627	25.863	0.478	4	138	13	129	123	27 duplicate
6529	58 [636; 4R-Acetamido-2,3	130	Trehalose	63	0.464	0.544	17.181	0.384	5	137	22	120	85	85 original
6465	58 [636; 4R-Acetamido-2,3	66	Glyceric acid-3-phosphate	64	0.439	0.739	15.604	0.471	6	136	7	135	55	30 original

13844	58 [636; 4R-Acetalamido-2,3	32	[728; N,N-Dimethyllysine methyl ester]	63	0.419	0.690	21,513	0.472	7	135	10	132	99	28 duplicate
14270	58 [636; 4R-Acetalamido-2,3	38	[596; N-Acetylglutamic acid (2TMS)]	64	0.417	0.623	15,239	0.534	8	134	14	128	50	9 duplicate
6458	58 [636; 4R-Acetalamido-2,3	59	Omithine; Arginine	64	0.414	0.835	27,048	0.494	9	133	2	140	127	22 original
6478	58 [636; 4R-Acetalamido-2,3	79	Glucose	64	0.412	0.195	22,580	0.460	10	132	4	98	106	33 original
10819	58 [636; 4R-Acetalamido-2,3	7	Threonine	64	0.395	0.778	16,882	0.512	11	131	5	137	61	14 duplicate
13735	58 [636; 4R-Acetalamido-2,3	31	[622; Parabanic acid (2TMS)]	64	0.386	0.575	20,048	0.436	12	130	16	126	86	43 duplicate
6497	58 [636; 4R-Acetalamido-2,3	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	64	0.365	0.425	26,838	0.393	13	129	30	112	126	76 original
11855	58 [636; 4R-Acetalamido-2,3	15	Alanine	64	0.353	0.322	9,002	0.409	14	128	34	108	10	62 duplicate
6463	58 [636; 4R-Acetalamido-2,3	64	[789; Tyramine (3TMS)]	63	0.335	0.327	14,808	0.351	15	127	33	109	46	120 original
12827	58 [636; 4R-Acetalamido-2,3	23	Homoserine	64	0.321	0.514	12,863	0.413	16	126	24	118	32	56 duplicate
13952	58 [636; 4R-Acetalamido-2,3	33	Methionine	64	0.313	0.551	12,910	0.425	17	124	21	121	33	52 duplicate
6522	58 [636; 4R-Acetalamido-2,3	123	[945; Galactofuranose-6-phosphate (7TMS)]	64	0.313	0.375	8,514	0.460	18	125	32	110	6	34 original
13625	58 [636; 4R-Acetalamido-2,3	30	[815; Ethyl-3-(2H)-thiophenone]	64	0.293	0.745	15,754	0.490	19	123	6	136	56	23 duplicate
10952	58 [636; 4R-Acetalamido-2,3	8	Isoleucine	55	0.292	0.721	10,222	0.556	20	122	8	134	18	5 duplicate
10414	58 [636; 4R-Acetalamido-2,3	4	Phosphoric acid	51	0.288	0.450	19,500	0.557	21	121	28	114	84	4 duplicate
6480	58 [636; 4R-Acetalamido-2,3	81	Tyrosine	64	0.279	0.707	16,756	0.499	23	119	9	133	60	12 original
14879	58 [636; 4R-Acetalamido-2,3	42	Glutamic acid	60	0.279	0.661	19,069	0.431	24	118	12	130	79	19 duplicate
14059	58 [636; 4R-Acetalamido-2,3	34	Aspartic acid	64	0.270	0.661	19,069	0.431	25	117	29	113	9	48 duplicate
11215	58 [636; 4R-Acetalamido-2,3	10	Glycine	64	0.261	0.445	8,683	0.390	25	117	29	113	9	79 duplicate
6503	58 [636; 4R-Acetalamido-2,3	104	[795; Erythritol (4TMS)]	63	0.247	0.299	14,332	0.409	26	116	36	106	43	61 original
6537	58 [636; 4R-Acetalamido-2,3	138	[674; Ergosterol (1TMS)]	46	0.227	0.271	23,813	0.392	27	115	39	103	114	78 original
6482	58 [636; 4R-Acetalamido-2,3	83	Sorbitol	58	0.223	0.570	8,849	0.550	28	114	18	124	8	6 original
6468	58 [636; 4R-Acetalamido-2,3	69	Arginine	60	0.219	0.525	10,208	0.505	29	113	23	119	17	17 original
6476	58 [636; 4R-Acetalamido-2,3	77	[826; beta-[[[5-methyl-2-thienyl)methyl]eneamino-benzeneacetic acid methyl ester]	62	0.210	0.665	16,212	0.483	30	112	11	131	59	25 original
10277	58 [636; 4R-Acetalamido-2,3	3	Ethanolamine	62	0.208	0.469	20,185	0.454	31	111	27	115	87	35 duplicate
13060	58 [636; 4R-Acetalamido-2,3	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	0.207	0.485	19,252	0.383	32	110	26	116	81	89 duplicate
14977	58 [636; 4R-Acetalamido-2,3	43	[548; Leucine (2TBS)]	60	0.206	0.197	11,954	0.381	33	109	43	99	26	91 duplicate
6517	58 [636; 4R-Acetalamido-2,3	118	[928; Glucopyranose-6-phosphate (6TMS)]	58	0.176	0.109	17,327	0.309	34	108	52	90	68	134 original
12349	58 [636; 4R-Acetalamido-2,3	19	Alanine (BP) (3TMS)	64	0.174	0.135	10,166	0.377	35	107	50	92	16	93 duplicate
14780	58 [636; 4R-Acetalamido-2,3	41	[639; Proline (2TMS)]	64	0.169	0.181	8,391	0.380	36	106	47	95	4	95 duplicate
6532	58 [636; 4R-Acetalamido-2,3	133	[855; Squalene]	64	0.168	0.285	13,517	0.402	37	105	38	104	35	69 original
6459	58 [636; 4R-Acetalamido-2,3	60	Glycerol-3-phosphate	64	0.166	0.514	9,387	0.472	38	104	25	117	12	29 original
14374	58 [636; 4R-Acetalamido-2,3	37	Phenylalanine	64	0.155	0.575	10,461	0.480	39	103	17	125	19	28 duplicate
6513	58 [636; 4R-Acetalamido-2,3	114	Fructose-6-phosphate	53	0.151	0.089	17,128	0.405	40	102	55	87	64	65 original
6535	58 [636; 4R-Acetalamido-2,3	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.132	0.290	6,936	0.265	41	101	37	105	1	140 original
15170	58 [636; 4R-Acetalamido-2,3	45	Homocysteine	61	0.117	0.214	31,782	0.377	42	100	41	101	138	88 duplicate
6512	58 [636; 4R-Acetalamido-2,3	113	Galactose-6-phosphate	62	0.108	0.031	18,400	0.428	43	99	59	83	73	50 original
6470	58 [636; 4R-Acetalamido-2,3	71	[731; Erythrose (3TMS)]	64	0.107	0.559	7,115	0.452	44	98	20	122	2	37 original
6530	58 [636; 4R-Acetalamido-2,3	131	[626; 5-Methylthiodenosine (3TMS)]	55	0.095	0.101	26,163	0.349	45	97	54	88	124	122 original
6466	58 [636; 4R-Acetalamido-2,3	67	Citric acid	64	0.094	0.593	11,513	0.428	46	96	15	127	23	51 original
15452	58 [636; 4R-Acetalamido-2,3	48	Asparagine	64	0.090	0.267	15,283	0.408	47	95	40	102	51	63 duplicate
6472	58 [636; 4R-Acetalamido-2,3	73	[708; Glucose methoxyamine (5TMS)]	57	0.081	0.105	19,347	0.404	48	94	53	89	83	67 original
10685	58 [636; 4R-Acetalamido-2,3	6	Glycerol	64	0.080	-0.032	29,179	0.353	49	93	64	78	135	115 duplicate
		124	[734; 1-Monocleoylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	59	0.079	0.193	33,362	0.352	50	92	45	97	140	117 original
6523	58 [636; 4R-Acetalamido-2,3		[772; D-Glucose (5TMS)]	62	0.065	-0.100	20,950	0.307	51	91	75	67	95	135 original
6479	58 [636; 4R-Acetalamido-2,3	80	[772; D-Glucose (5TMS)]	64	0.040	0.192	16,950	0.362	52	90	46	96	62	107 original
6507	58 [636; 4R-Acetalamido-2,3	108	Octadecanoic acid	64	0.040	0.017	25,224	0.307	53	89	61	120	138	107 original
6538	58 [636; 4R-Acetalamido-2,3	139	[700; Ergosta-5,7-dien-3-ol]	38	0.010	0.017	25,224	0.307	53	89	61	120	138	107 original
6493	58 [636; 4R-Acetalamido-2,3	94	Hexadecanoic acid	64	0.004	0.181	11,849	0.362	54	88	48	94	24	108 original
15725	58 [636; 4R-Acetalamido-2,3	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.002	0.378	29,099	0.497	55	87	31	111	133	20 duplicate

6508	58 [636; 4R-Acetylido-2,3	109	Octadecanoic acid	64	-0.015	0.199	14.386	0.351	56	86	42	100	44	118 original
14165	58 [636; 4R-Acetylido-2,3	35	Pyroglutamic acid	64	-0.018	-0.099	28.874	0.347	57	85	74	68	132	123 duplicate
6505	58 [636; 4R-Acetylido-2,3	106	Threitol (4TMS)	63	-0.029	-0.103	15.528	0.471	58	84	76	68	54	31 original
6471	58 [636; 4R-Acetylido-2,3	72	[919; D-Xylopyranose (4TMS)]	63	-0.030	-0.068	18.686	0.368	59	83	71	71	77	102 original
15544	58 [636; 4R-Acetylido-2,3	49	[877; Pyrophosphoric acid (4TMS)]	64	-0.032	-0.059	30.200	0.339	60	82	68	74	137	125 duplicate
6460	58 [636; 4R-Acetylido-2,3	61	[NA]	64	-0.035	0.070	14.075	0.349	61	81	56	86	40	121 original
6536	58 [636; 4R-Acetylido-2,3	137	Ergosterol	49	-0.040	0.159	11.350	0.353	62	80	49	93	22	114 original
6539	58 [636; 4R-Acetylido-2,3	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	49	-0.041	-0.134	25.008	0.398	63	79	80	62	119	71 original
6469	58 [636; 4R-Acetylido-2,3	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	-0.044	-0.034	10.655	0.374	64	78	65	77	20	97 original
6510	58 [636; 4R-Acetylido-2,3	111	[583; Erythritol (4TMS)]	42	-0.045	0.020	27.999	0.266	65	77	60	82	130	138 original
6495	58 [636; 4R-Acetylido-2,3	98	myo-Inositol	49	-0.054	-0.060	29.158	0.379	66	76	69	73	134	94 original
6475	58 [636; 4R-Acetylido-2,3	76	Fructose	58	-0.056	-0.149	17.379	0.330	67	75	82	60	69	130 original
6520	58 [636; 4R-Acetylido-2,3	121	[657; Erythritol (4TMS)]	55	-0.057	-0.021	23.634	0.383	68	74	63	78	112	88 original
6486	58 [636; 4R-Acetylido-2,3	87	[945; beta-D-Glucopyranose (5TMS)]	62	-0.060	-0.153	24.648	0.370	69	73	84	58	117	101 original
12227	58 [636; 4R-Acetylido-2,3	18	[590; 1-Acetyl-2-thiohydantoin]	64	-0.064	-0.050	12.149	0.357	70	72	67	75	27	112 duplicate
6516	58 [636; 4R-Acetylido-2,3	117	[724; Glycerol (3TMS)]	56	-0.077	-0.092	17.028	0.420	71	71	72	70	63	56 original
6514	58 [636; 4R-Acetylido-2,3	115	Glucose-6-phosphate	62	-0.079	-0.114	14.927	0.346	72	70	77	65	47	124 original
6524	58 [636; 4R-Acetylido-2,3	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	-0.092	-0.120	21.659	0.339	73	69	78	64	100	128 original
6494	58 [636; 4R-Acetylido-2,3	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	-0.094	0.053	28.736	0.289	74	68	57	85	131	137 original
6484	58 [636; 4R-Acetylido-2,3	85	[529; Methylcitric acid (4TMS)]	48	-0.098	-0.129	13.984	0.589	75	67	79	63	39	1 original
6477	58 [636; 4R-Acetylido-2,3	78	Mannose	62	-0.099	-0.216	21.112	0.366	76	66	87	55	97	103 original
6525	58 [636; 4R-Acetylido-2,3	126	[559; Erythritol (4TMS)]	45	-0.107	0.044	15.519	0.449	77	65	58	84	53	40 original
6515	58 [636; 4R-Acetylido-2,3	116	[882; Pseudouridine (5TMS)]	30	-0.108	-0.413	15.412	0.509	78	64	113	29	52	15 original
6467	58 [636; 4R-Acetylido-2,3	68	[570; Hypoxanthine (2TMS)]	20	-0.116	0.321	19.334	0.403	79	63	35	107	82	68 original
14680	58 [636; 4R-Acetylido-2,3	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.117	-0.204	22.090	0.430	80	62	86	56	105	49 duplicate
6509	58 [636; 4R-Acetylido-2,3	110	[715; Erythritol (4TMS)]	54	-0.119	-0.141	20.717	0.497	81	61	81	61	93	21 original
6540	58 [636; 4R-Acetylido-2,3	141	Lanosta-8,24-dien-3-beta-ol	61	-0.122	-0.173	24.936	0.418	82	60	85	57	118	57 original
12470	20 [619; 2-(3',4'-Bishydroxyphenyl)-2-oxethylamine (4TMS)]			31	-0.127	-0.322	23.030	0.518	83	59	103	39	109	13 duplicate
15902	58 [636; 4R-Acetylido-2,3	53	Glycerol-2-phosphate	64	-0.128	-0.228	21.900	0.359	84	58	91	51	101	111 duplicate
10050	58 [636; 4R-Acetylido-2,3	5	Leucine	45	-0.133	0.120	18.538	0.572	85	57	51	91	75	2 duplicate
15074	58 [636; 4R-Acetylido-2,3	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	-0.146	-0.152	15.129	0.399	86	56	83	59	48	70 duplicate
13175	58 [636; 4R-Acetylido-2,3	26	Citramalic acid	64	-0.151	-0.268	8.297	0.383	87	55	97	45	3	90 duplicate
6473	58 [636; 4R-Acetylido-2,3	74	[912; Tetradecanoic acid (1TMS)]	64	-0.153	-0.035	18.724	0.371	88	54	68	76	78	98 original
6521	58 [636; 4R-Acetylido-2,3	122	[644; Erythritol (4TMS)]	52	-0.163	-0.219	25.281	0.454	89	53	89	53	121	38 original
6481	58 [636; 4R-Acetylido-2,3	82	Lysine	39	-0.177	-0.231	12.758	0.558	90	52	92	50	30	3 original
6500	58 [636; 4R-Acetylido-2,3	101	[832; Dopamine (4TMS)]	64	-0.183	-0.562	18.382	0.451	91	51	136	6	72	38 original
15914	58 [636; 4R-Acetylido-2,3	52	[NA]	46	-0.186	-0.064	26.411	0.438	92	50	70	72	125	41 duplicate
13402	58 [636; 4R-Acetylido-2,3	28	Malic acid	64	-0.198	-0.384	11.310	0.412	94	48	108	34	21	59 duplicate
6531	58 [636; 4R-Acetylido-2,3	132	[895; Isomaltose methoxyamine (8TMS)]	42	-0.203	-0.416	23.632	0.282	95	47	115	27	111	139 original
12590	58 [636; 4R-Acetylido-2,3	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	-0.203	-0.362	9.939	0.393	96	46	105	37	14	75 duplicate
6485	58 [636; 4R-Acetylido-2,3	86	[783; D-Galactono-1,4-lactone (4TMS)]	61	-0.207	-0.300	21.439	0.432	97	45	101	41	98	47 original
6490	58 [636; 4R-Acetylido-2,3	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	-0.218	-0.643	23.966	0.507	98	44	139	3	115	18 original
6518	58 [636; 4R-Acetylido-2,3	119	[931; myo-Inositol-2-phosphate (7TMS)]	64	-0.219	-0.265	14.623	0.352	99	43	96	46	45	116 original
15359	58 [636; 4R-Acetylido-2,3	47	[NA]	64	-0.225	-0.385	18.481	0.435	100	42	109	33	74	44 duplicate
11729	58 [636; 4R-Acetylido-2,3	14	Fumaric acid	64	-0.232	-0.415	20.458	0.392	101	41	114	28	91	77 duplicate
6526	58 [636; 4R-Acetylido-2,3	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	59	-0.233	-0.291	12.176	0.194	102	40	100	42	28	141 original
6519	58 [636; 4R-Acetylido-2,3	120	[945; Uridine (3TMS)]	34	-0.234	-0.236	9.970	0.334	103	39	93	49	15	127 original
6506	58 [636; 4R-Acetylido-2,3	107	9-Z-Octadecanoic acid	64	-0.237	-0.095	8.551	0.333	104	38	73	69	7	128 original
6461	58 [636; 4R-Acetylido-2,3	62	[812; D-Xylofuranose (4TMS)]	64	-0.243	-0.290	9.300	0.385	105	37	99	43	11	82 original
16233	58 [636; 4R-Acetylido-2,3	56	[829; Orolic acid (3TMS)]	64	-0.251	-0.381	21.995	0.394	106	36	106	36	103	73 duplicate

12709	58 [636; 4R-Acetylido-2,3	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	-0,252	-0,485	22,628	0,395	107	35	126	16	108	72 duplicate
6501	58 [636; 4R-Acetylido-2,3	102	[904; Galactose methoxyamine (5TMS)]	64	-0,253	-0,260	17,216	0,364	108	34	95	47	67	104 original
6502	58 [636; 4R-Acetylido-2,3	103	[648; Ethylamine (2TMS)]	63	-0,259	-0,555	20,200	0,449	109	33	135	7	88	39 original
6498	58 [636; 4R-Acetylido-2,3	89	[775; Dopamine (4TMS)]	35	-0,271	-0,221	22,018	0,470	110	32	90	52	104	32 original
6462	58 [636; 4R-Acetylido-2,3	63	Glutamine	52	-0,273	0,002	21,080	0,318	111	31	62	80	98	132 original
11602	58 [636; 4R-Acetylido-2,3	13	Uracil	64	-0,286	-0,498	14,232	0,425	112	30	127	15	42	53 duplicate
6499	58 [636; 4R-Acetylido-2,3	100	[857; Mannitol (6TMS)]	64	-0,287	-0,383	11,859	0,351	113	28	107	35	25	119 original
14477	58 [636; 4R-Acetylido-2,3	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0,287	-0,479	13,889	0,394	114	29	123	19	38	74 duplicate
6533	58 [636; 4R-Acetylido-2,3	134	Isomaltose	64	-0,290	-0,434	20,353	0,389	115	27	118	24	90	80 original
14579	58 [636; 4R-Acetylido-2,3	39	[828; 1-Phenylethanol (1TMS)]	63	-0,280	-0,461	17,809	0,380	116	26	120	22	70	92 duplicate
6487	58 [636; 4R-Acetylido-2,3	88	Gluconic acid	64	-0,291	-0,473	15,849	0,437	117	25	122	20	58	42 original
11345	58 [636; 4R-Acetylido-2,3	11	Succinic acid	64	-0,300	-0,410	12,878	0,384	118	24	112	30	31	86 duplicate
12104	58 [636; 4R-Acetylido-2,3	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	-0,305	-0,455	13,278	0,404	119	23	119	23	34	66 duplicate
16075	58 [636; 4R-Acetylido-2,3	55	[612; 4-Aminobutyric acid (2TBS)]	43	-0,318	-0,480	32,562	0,539	120	22	124	18	139	8 duplicate
12944	58 [636; 4R-Acetylido-2,3	24	[725; 2-Ketooctanoic acid (2TMS)]	64	-0,329	-0,480	21,934	0,406	121	20	125	17	102	64 duplicate
11980	58 [636; 4R-Acetylido-2,3	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	-0,329	-0,512	12,418	0,425	122	21	130	12	28	54 duplicate
6528	58 [636; 4R-Acetylido-2,3	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	-0,334	-0,431	20,225	0,355	123	19	117	25	89	113 original
6489	58 [636; 4R-Acetylido-2,3	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	64	-0,336	-0,331	13,780	0,333	124	17	104	38	37	129 original
15265	58 [636; 4R-Acetylido-2,3	46	Arabinose	64	-0,336	-0,407	19,964	0,389	125	18	110	32	85	81 duplicate
6464	58 [636; 4R-Acetylido-2,3	65	[646; 3-Deoxyglucitol (5TMS)]	63	-0,341	-0,420	23,752	0,383	126	18	116	26	113	87 original
13514	58 [636; 4R-Acetylido-2,3	29	Erythritol	64	-0,342	-0,514	15,772	0,424	127	15	131	11	57	55 duplicate
6534	58 [636; 4R-Acetylido-2,3	135		64	-0,343	-0,219	8,404	0,360	128	14	88	54	5	110 original
15635	58 [636; 4R-Acetylido-2,3	50	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	61	-0,350	-0,527	30,118	0,433	129	13	134	8	138	48 duplicate
6511	58 [636; 4R-Acetylido-2,3	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	-0,354	-0,321	27,538	0,384	130	12	102	40	128	84 original
6496	58 [636; 4R-Acetylido-2,3	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	-0,373	-0,595	20,857	0,488	131	11	137	5	94	24 original
6527	58 [636; 4R-Acetylido-2,3	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	-0,414	-0,472	13,644	0,321	132	10	121	21	36	131 original
16317	58 [636; 4R-Acetylido-2,3	57	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55	-0,418	-0,408	19,120	0,384	133	9	111	31	80	105 duplicate
6491	58 [636; 4R-Acetylido-2,3	92	[680; Glycerol-2-phosphate (4TMS)]	54	-0,423	-0,274	17,208	0,318	134	8	98	44	66	133 original
11474	58 [636; 4R-Acetylido-2,3	12	Glyceric acid	63	-0,425	-0,520	22,615	0,370	135	7	132	10	107	100 duplicate
6498	58 [636; 4R-Acetylido-2,3	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	-0,459	-0,523	18,844	0,361	136	6	133	9	76	108 original
15989	58 [636; 4R-Acetylido-2,3	54	[NA]	55	-0,491	-0,503	23,151	0,384	137	5	129	13	110	83 duplicate
6492	58 [636; 4R-Acetylido-2,3	93	[607; Putrescine (4TMS)]	60	-0,507	-0,500	27,704	0,433	138	4	128	14	129	45 original
10000	58 [636; 4R-Acetylido-2,3	1	[938; Sulfuric acid (2TMS)]	36	-0,552	-0,619	15,175	0,371	139	3	138	4	49	99 duplicate
6504	58 [636; 4R-Acetylido-2,3	105	[705; 2-Ketogluconic acid (5TMS)]	48	-0,590	-0,703	17,903	0,411	140	2	140	2	71	60 original
6483	58 [636; 4R-Acetylido-2,3	84	Mannitol	62	-0,608	-0,793	24,286	0,530	141	1	141	1	116	11 original
6550	59 Ornithine; Arginine	69	Arginine	60	0,771	0,937	23,872	0,620	1	141	1	141	29	1 original
6563	59 Ornithine; Arginine	82	Lysine	39	0,757	0,900	24,401	0,584	2	140	5	137	31	5 original
6558	59 Ornithine; Arginine	77	[826; beta-[[[5-methyl-2-ithienyl)methyl]amino]-benzenesulfonic acid methyl ester]	62	0,757	0,912	15,969	0,544	3	139	4	138	13	11 original
6562	59 Ornithine; Arginine	81	Tyrosine	64	0,743	0,830	10,705	0,526	4	138	12	130	7	18 original
14880	59 Ornithine; Arginine	42	Glutamic acid	60	0,740	0,931	19,492	0,619	5	137	2	140	20	2 duplicate
13826	59 Ornithine; Arginine	30	[915; Ethyl-3(2H)-thiophenone]	64	0,708	0,920	14,100	0,501	6	136	3	139	11	39 duplicate
13953	59 Ornithine; Arginine	33	Methionine	64	0,690	0,810	37,215	0,519	7	135	16	128	76	21 duplicate
13845	59 Ornithine; Arginine	32	[728; N,N-Dimethyllysine methyl ester]	63	0,677	0,873	46,485	0,572	8	134	6	136	120	7 duplicate
11216	59 Ornithine; Arginine	10	Glycine	64	0,675	0,757	24,257	0,502	9	133	21	121	30	37 duplicate
11085	59 Ornithine; Arginine	9	Proline	63	0,649	0,858	21,000	0,511	10	132	8	134	25	27 duplicate
10278	59 Ornithine; Arginine	3	Ethanolamine	62	0,645	0,774	45,438	0,481	11	131	19	123	113	53 duplicate
13736	59 Ornithine; Arginine	31	[822; Parabenic acid (2TMS)]	64	0,603	0,738	46,011	0,504	12	130	24	118	117	34 duplicate

15726	59 Ornithine; Arginine	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44 0.600	0.868	51.028	0.577	13	129	7	135	131	6 duplicate
14375	59 Ornithine; Arginine	37 Phenylalanine	64 0.600	0.792	16.784	0.495	14	128	18	124	18	42 duplicate
10953	59 Ornithine; Arginine	8 Isoleucine	55 0.593	0.727	27.626	0.537	15	127	25	117	40	15 duplicate
14060	59 Ornithine; Arginine	34 Aspartic acid	64 0.590	0.853	9.645	0.515	16	126	9	133	5	24 duplicate
15453	59 Ornithine; Arginine	48 Asparagine	64 0.560	0.873	38.072	0.503	17	125	28	114	81	35 duplicate
6548	59 Ornithine; Arginine	67 Citric acid	64 0.548	0.767	17.786	0.437	18	124	20	122	15	82 original
10140	59 Ornithine; Arginine	2 Serine	62 0.545	0.829	29.417	0.539	19	123	13	129	47	13 duplicate
10551	59 Ornithine; Arginine	5 Leucine	45 0.537	0.819	38.973	0.595	20	122	14	128	85	4 duplicate
13290	59 Ornithine; Arginine	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53 0.509	0.803	48.523	0.551	21	121	17	125	126	9 duplicate
15171	59 Ornithine; Arginine	45 Homocysteine	61 0.507	0.548	57.303	0.429	22	120	35	107	139	86 duplicate
12828	59 Ornithine; Arginine	23 Homoserine	64 0.505	0.722	37.137	0.502	23	119	26	116	75	38 duplicate
6541	59 Ornithine; Arginine	60 Glycerol-3-phosphate	64 0.502	0.861	20.388	0.455	24	118	30	112	24	67 original
6547	59 Ornithine; Arginine	68 Glyceral acid-3-phosphate	64 0.500	0.740	41.579	0.455	25	117	23	119	101	68 original
10820	59 Ornithine; Arginine	7 Threonine	64 0.497	0.819	11.351	0.498	26	116	15	127	8	40 duplicate
16076	59 Ornithine; Arginine	55 [612; 4-Aminobutyric acid (2TBS)]	43 0.488	0.666	53.131	0.565	27	115	29	113	135	8 duplicate
6556	59 Ornithine; Arginine	75 Lysine	64 0.460	0.850	3.456	0.534	28	114	10	132	1	16 original
6612	59 Ornithine; Arginine	131 [626; 5-Methylthiodenosine (3TMS)]	55 0.434	0.375	49.984	0.396	29	113	45	97	130	100 original
6576	59 Ornithine; Arginine	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50 0.416	0.425	51.854	0.377	30	112	41	101	133	110 original
16401	59 Ornithine; Arginine	[636; 4R-Acetyl-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64 0.414	0.835	27.048	0.494	31	111	11	131	38	44 duplicate
6570	59 Ornithine; Arginine	89 [775; Dopamine (4TMS)]	35 0.402	0.655	39.002	0.549	32	110	31	111	86	10 original
6579	59 Ornithine; Arginine	98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	48 0.399	0.582	49.662	0.512	33	109	33	109	129	26 original
6542	59 Ornithine; Arginine	61 [NA]	64 0.397	0.431	38.732	0.394	34	108	40	102	84	107 original
15545	59 Ornithine; Arginine	49 [877; Pyrophosphoric acid (4TMS)]	64 0.388	0.283	54.605	0.378	35	107	48	94	137	109 duplicate
13061	59 Ornithine; Arginine	25 [709; 2,5-Diaminovalerolactam (2TMS)]	48 0.372	0.633	39.350	0.464	36	106	32	110	88	60 duplicate
6549	59 Ornithine; Arginine	68 [570; Hypoxanthine (2TMS)]	20 0.368	0.745	35.163	0.544	37	105	22	120	64	12 original
6617	59 Ornithine; Arginine	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17 0.368	0.548	19.177	0.291	38	104	36	106	19	139 original
12471	59 Ornithine; Arginine	20 [619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	31 0.355	0.714	40.806	0.599	39	103	27	115	96	3 duplicate
14271	59 Ornithine; Arginine	36 [596; N-Acetylglutamic acid (2TMS)]	64 0.354	0.560	14.191	0.485	40	102	34	108	12	51 duplicate
14978	59 Ornithine; Arginine	43 [548; Leucine (2TBS)]	60 0.325	0.406	36.010	0.396	41	101	43	99	68	101 duplicate
6589	59 Ornithine; Arginine	108 Octadecanoic acid	64 0.261	0.321	42.173	0.374	42	100	47	95	103	112 original
6552	59 Ornithine; Arginine	71 [731; Erythrose (3TMS)]	64 0.247	0.537	30.189	0.459	43	99	37	105	51	63 original
6605	59 Ornithine; Arginine	124 [734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]	59 0.220	0.276	58.624	0.339	44	98	49	93	140	132 original
6611	59 Ornithine; Arginine	130 Trehalose	63 0.219	0.386	11.863	0.339	45	97	44	98	9	131 original
15815	59 Ornithine; Arginine	52 [NA]	46 0.163	0.327	47.442	0.516	46	96	46	96	123	23 duplicate
6544	59 Ornithine; Arginine	63 Glutamine	52 0.143	0.421	40.856	0.457	47	95	42	100	98	65 original
10415	59 Ornithine; Arginine	4 Phosphoric acid	51 0.120	0.450	6.629	0.473	48	94	39	103	2	54 duplicate
6600	59 Ornithine; Arginine	119 [931; myo-Inositol-2-phosphate (7TMS)]	64 0.107	0.007	37.616	0.368	49	93	57	85	79	118 original
6618	59 Ornithine; Arginine	137 Ergosterol	64 0.090	0.209	31.609	0.355	50	92	50	92	55	123 original
6568	59 Ornithine; Arginine	107 9-(Z)-Octadecanoic acid	64 0.085	0.102	28.003	0.354	51	91	54	88	42	124 original
6619	59 Ornithine; Arginine	138 [674; Ergosterol (1TMS)]	46 0.067	0.111	46.336	0.319	52	90	53	89	119	137 original
6820	59 Ornithine; Arginine	139 [700; Ergosta-5,7-dien-3-ol]	38 0.053	0.140	45.570	0.258	53	89	52	90	115	141 original
6545	59 Ornithine; Arginine	64 [789; Tyramine (3TMS)]	63 0.040	0.086	40.018	0.342	54	88	55	87	91	129 original
6614	59 Ornithine; Arginine	133 [655; Squalene]	64 0.028	0.168	38.320	0.364	55	87	51	91	82	118 original
6564	59 Ornithine; Arginine	83 Sorbitol	59 -0.007	0.536	21.576	0.483	56	86	38	104	26	52 original
6575	59 Ornithine; Arginine	94 Hexadecanoic acid	64 -0.013	0.008	23.224	0.338	57	85	56	86	27	133 original
6622	59 Ornithine; Arginine	141 Lanosta-8,24-dien-3-beta-ol	61 -0.019	-0.116	49.621	0.365	58	84	64	78	128	117 original
11856	59 Ornithine; Arginine	15 Alanine	64 -0.021	-0.035	25.711	0.461	59	83	59	83	33	62 duplicate
6560	59 Ornithine; Arginine	78 Glucose	64 -0.024	-0.240	13.129	0.454	60	82	72	70	10	70 original



15903	59 Ornithine; Arginine	53	Glycerol-2-phosphate	64	-0.028	-0.123	47.364	0.328	61	81	65	77	122	135 duplicate
6590	59 Ornithine; Arginine	109	Octadecanoic acid	64	-0.032	-0.030	26.418	0.345	62	80	58	84	35	128 original
6592	59 Ornithine; Arginine	111	[583; Erythritol (4TMS)]	42	-0.057	-0.053	48.684	0.260	63	79	61	81	127	140 original
6593	59 Ornithine; Arginine	72	[919; D-Xylopyranose (4TMS)]	63	-0.061	-0.045	43.015	0.353	64	78	60	82	107	125 original
6571	59 Ornithine; Arginine	90	[910; 9-(Z)-Hexadecanoic acid (1TMS)]	64	-0.077	-0.167	37.340	0.328	65	77	68	74	77	138 original
6574	59 Ornithine; Arginine	93	[607; Putrescine (4TMS)]	60	-0.078	-0.281	51.421	0.404	66	76	73	69	132	97 original
6621	59 Ornithine; Arginine	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	49	-0.080	-0.160	47.913	0.364	67	75	67	75	125	120 original
6599	59 Ornithine; Arginine	118	[928; Glucopyranose-6-phosphate (6TMS)]	58	-0.103	-0.128	40.848	0.329	68	74	66	76	97	134 original
6604	59 Ornithine; Arginine	123	[945; Galactofuranose-6-phosphate (7TMS)]	64	-0.113	-0.062	32.462	0.432	69	73	62	80	57	85 original
6608	59 Ornithine; Arginine	127	[777; Fructose-6-phosphate methoxymine (6TMS)]	39	-0.131	-0.302	29.028	0.300	70	72	76	66	45	138 original
6607	59 Ornithine; Arginine	126	[559; Erythritol (4TMS)]	45	-0.143	-0.102	34.682	0.452	71	71	63	78	62	72 original
6595	59 Ornithine; Arginine	114	Fructose-6-phosphate	53	-0.173	-0.317	40.502	0.404	72	70	79	63	94	96 original
6565	59 Ornithine; Arginine	84	Mannitol	62	-0.173	-0.655	19.522	0.492	73	69	117	25	21	47 original
6585	59 Ornithine; Arginine	104	[795; Erythritol (4TMS)]	63	-0.183	-0.173	39.489	0.410	74	68	69	73	90	94 original
6594	59 Ornithine; Arginine	113	Galactose-6-phosphate	62	-0.217	-0.365	43.080	0.432	75	67	84	58	108	84 original
6566	59 Ornithine; Arginine	85	[529; Methylenic acid (4TMS)]	48	-0.230	-0.543	36.367	0.537	76	68	103	39	70	14 original
14781	59 Ornithine; Arginine	41	[639; Proline (2TMS)]	64	-0.231	-0.193	29.788	0.361	77	65	70	72	49	121 duplicate
6577	59 Ornithine; Arginine	96	myo-Inositol	49	-0.253	-0.195	52.282	0.369	78	64	71	71	134	115 original
6616	59 Ornithine; Arginine	135												
6555	59 Ornithine; Arginine	74	[902; Melibiose (8TMS); alpha-D-Gal(1,6)-D-Glc (8TMS)]	64	-0.275	-0.291	30.288	0.391	79	62	74	68	52	106 original
15360	59 Ornithine; Arginine	47	[912; Tetradecanoic acid (1TMS)]	64	-0.275	-0.300	42.733	0.407	80	63	75	67	106	85 original
15075	59 Ornithine; Arginine	44	[910; 2-Ketogluconic acid methoxymine (4TMS)]	50	-0.280	-0.351	40.428	0.399	81	61	85	57	93	88 duplicate
12350	59 Ornithine; Arginine	19	Alanine (BP) (3TMS)	64	-0.288	-0.310	32.715	0.396	83	59	77	65	58	90 duplicate
12228	59 Ornithine; Arginine	18	[590; 1-Acetyl-2-thiohydantoin]	64	-0.306	-0.338	36.349	0.371	84	58	81	61	69	114 duplicate
6587	59 Ornithine; Arginine	116	[882; Pseudouridine (5TMS)]	30	-0.324	-0.317	32.030	0.451	85	57	80	62	56	73 original
6613	59 Ornithine; Arginine	132	[895; Isomaltose methoxymine (8TMS)]	42	-0.326	-0.608	41.817	0.372	86	56	109	33	102	113 original
6583	59 Ornithine; Arginine	102	[904; Galactose methoxymine (5TMS)]	64	-0.339	-0.392	42.277	0.415	87	55	86	56	104	92 original
10686	59 Ornithine; Arginine	6	Glycerol	64	-0.341	-0.458	8.977	0.395	88	54	92	50	3	103 duplicate
6561	59 Ornithine; Arginine	80	[772; D-Glucose (5TMS)]	62	-0.344	-0.472	19.636	0.364	89	53	94	48	22	119 original
6602	59 Ornithine; Arginine	121	[657; Erythritol (4TMS)]	55	-0.349	-0.347	46.847	0.383	90	51	82	60	121	108 original
6609	59 Ornithine; Arginine	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	-0.349	-0.475	29.512	0.340	91	52	95	47	48	130 original
6603	59 Ornithine; Arginine	122	[644; Erythritol (4TMS)]	52	-0.359	-0.442	46.259	0.429	92	50	91	51	118	87 original
6598	59 Ornithine; Arginine	117	[724; Glyceral (3TMS)]	56	-0.360	-0.419	39.223	0.423	93	49	88	54	87	89 original
6591	59 Ornithine; Arginine	100	[857; Mannitol (6TMS)]	64	-0.361	-0.508	34.948	0.426	94	48	98	44	63	88 original
6591	59 Ornithine; Arginine	110	[715; Erythritol (4TMS)]	54	-0.375	-0.434	41.501	0.466	95	47	90	52	100	57 original
14166	59 Ornithine; Arginine	35	Pyrogalluric acid	64	-0.376	-0.503	9.727	0.442	96	46	97	45	6	77 duplicate
6593	59 Ornithine; Arginine	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	-0.388	-0.467	53.359	0.391	97	45	93	49	136	105 original
6554	59 Ornithine; Arginine	73	[708; Glucose methoxymine (5TMS)]	57	-0.405	-0.316	42.691	0.456	98	44	78	64	105	68 original
6572	59 Ornithine; Arginine	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	-0.406	-0.678	41.324	0.453	99	43	121	21	99	71 original
6596	59 Ornithine; Arginine	115	Glucose-6-phosphate	62	-0.407	-0.496	19.845	0.437	100	42	96	46	23	83 original
6578	59 Ornithine; Arginine	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	-0.430	-0.654	28.122	0.439	101	41	116	26	44	79 original
6601	59 Ornithine; Arginine	120	[945; Uridine (3TMS)]	54	-0.433	-0.428	27.864	0.504	102	40	89	53	41	33 original
14681	59 Ornithine; Arginine	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.434	-0.547	9.556	0.465	103	39	104	38	4	59 duplicate
13176	59 Ornithine; Arginine	26	Citramalic acid	64	-0.441	-0.541	26.030	0.449	104	38	102	40	34	75 duplicate
6582	59 Ornithine; Arginine	101	[832; Dopamine (4TMS)]	64	-0.447	-0.643	39.376	0.454	105	37	113	29	89	69 original
13403	59 Ornithine; Arginine	106	[733; Threitol (4TMS)]	62	-0.448	-0.518	37.845	0.523	106	38	100	42	80	20 original
6557	59 Ornithine; Arginine	28	Malic acid	64	-0.461	-0.651	34.323	0.494	108	34	115	27	61	45 duplicate
6568	59 Ornithine; Arginine	76	Fructose	64	-0.463	-0.569	23.641	0.439	109	33	106	36	28	80 original
6586	59 Ornithine; Arginine	87	[945; beta-D-Glucopyranose (5TMS)]	62	-0.488	-0.572	18.030	0.441	110	32	107	35	16	78 original
		105	[705; 2-Ketogluconic acid (5TMS)]	48	-0.491	-0.644	31.302	0.374	111	31	114	28	54	111 original

12591	59 Ornithine; Arginine	64 -0.500	-0.643	26,740	0.466	112	30	112	30	38	58 duplicate
6573	59 Ornithine; Arginine	54 -0.502	-0.510	37,435	0.348	113	29	99	43	78	127 original
6559	59 Ornithine; Arginine	62 -0.503	-0.594	44,779	0.399	114	28	108	34	110	89 original
6584	59 Ornithine; Arginine	63 -0.507	-0.870	38,623	0.494	115	27	119	23	83	48 original
10001	59 Ornithine; Arginine	36 -0.508	-0.634	29,905	0.352	116	26	111	31	50	128 duplicate
6608	59 Ornithine; Arginine	64 -0.514	-0.554	18,730	0.416	117	25	105	37	17	91 original
12710	59 Ornithine; Arginine	52 -0.519	-0.695	45,198	0.468	118	24	128	16	112	58 duplicate
11475	59 Ornithine; Arginine	63 -0.522	-0.692	47,580	0.463	119	23	125	17	124	61 duplicate
11730	59 Ornithine; Arginine	64 -0.537	-0.691	45,725	0.496	120	22	124	18	116	41 duplicate
6580	59 Ornithine; Arginine	41 -0.541	-0.690	38,951	0.411	121	21	123	19	73	93 original
6551	59 Ornithine; Arginine	57 -0.561	-0.408	24,548	0.394	122	20	87	55	32	104 original
14478	59 Ornithine; Arginine	64 -0.562	-0.729	37,132	0.504	123	19	131	11	74	22 duplicate
13515	59 Ornithine; Arginine	64 -0.577	-0.737	40,362	0.516	124	18	135	7	92	30 duplicate
16234	59 Ornithine; Arginine	64 -0.591	-0.702	45,191	0.506	125	17	127	15	111	28 original
6587	59 Ornithine; Arginine	61 -0.595	-0.725	35,857	0.510	126	16	129	13	68	30 duplicate
11346	59 Ornithine; Arginine	64 -0.596	-0.669	36,449	0.471	127	15	118	24	71	55 duplicate
6543	59 Ornithine; Arginine	64 -0.605	-0.630	29,073	0.450	128	14	110	32	46	74 original
12105	59 Ornithine; Arginine	17 [700; 2-methyl-1,2-propanediol (2TMS)]	-0.708	28,068	0.506	129	13	128	14	43	31 duplicate
14580	59 Ornithine; Arginine	39 [829; 1-Phenylethanol (1TMS)]	-0.736	34,206	0.490	130	12	133	8	60	50 duplicate
6815	59 Ornithine; Arginine	134 Isomaltose	-0.744	27,442	0.492	131	11	138	6	39	48 original
16318	57 [757; 2-Desoxy-pentos-3-yose dimethoxyamine (2TMS)]	55 -0.624	-0.678	35,713	0.437	132	10	122	20	65	81 duplicate
15980	59 Ornithine; Arginine	55 -0.631	-0.672	44,231	0.447	133	9	120	22	109	76 duplicate
6569	59 Ornithine; Arginine	64 -0.633	-0.744	35,962	0.503	134	8	137	5	67	38 original
6610	59 Ornithine; Arginine	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	-0.726	40,536	0.458	135	7	130	12	95	64 original
12945	59 Ornithine; Arginine	24 [725; 2-Ketoclanolic acid (2TMS)]	-0.766	16,287	0.532	136	6	138	4	14	17 duplicate
11981	59 Ornithine; Arginine	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	-0.771	26,932	0.525	137	5	139	3	37	19 duplicate
11803	59 Ornithine; Arginine	13 Uracil	-0.773	30,407	0.507	138	4	140	2	53	29 duplicate
15266	59 Ornithine; Arginine	46 Arabinose	-0.736	36,523	0.495	139	3	134	8	72	43 duplicate
6546	59 Ornithine; Arginine	65 [646; 3-Deoxyglucitol (5TMS)]	-0.732	45,486	0.491	140	2	132	10	114	49 original
15636	59 Ornithine; Arginine	50 [746; Ribonic acid-1,4-lactone (3TMS)]	-0.777	54,881	0.514	141	1	141	1	138	25 duplicate
6628	60 Glycerol-3-phosphate	67 Citric acid	0.895	3,687	0.591	1	141	1	141	2	4 original
14378	60 Glycerol-3-phosphate	37 Phenylalanine	0.855	2,747	0.565	2	140	3	139	1	9 duplicate
6643	60 Glycerol-3-phosphate	81 Tyrosine	0.860	13,853	0.596	3	139	2	140	34	3 original
10278	60 Glycerol-3-phosphate	3 Ethanolamine	0.817	25,702	0.554	4	138	4	138	106	14 duplicate
6639	60 Glycerol-3-phosphate	77 [826; beta-[(S-methyl-2-thienyl)methylethylamino]-benzeneacetic acid methyl ester]	0.790	12,045	0.502	5	137	5	137	25	46 original
6633	60 Glycerol-3-phosphate	71 [731; Erythrose (3TMS)]	0.780	10,259	0.517	6	136	6	136	18	31 original
6630	60 Glycerol-3-phosphate	68 [570; Hypoxanthine (2TMS)]	0.689	24,536	0.533	7	135	8	134	101	23 original
10821	60 Glycerol-3-phosphate	7 Threonine	0.736	9,617	0.462	8	134	7	135	11	74 duplicate
14881	60 Glycerol-3-phosphate	42 Glutamic acid	0.687	14,432	0.461	9	133	9	133	41	78 duplicate
11217	60 Glycerol-3-phosphate	10 Glycine	0.822	7,364	0.523	10	132	16	128	5	29 duplicate
16484	60 Glycerol-3-phosphate	59 Ornithine; Arginine	0.661	20,388	0.455	11	131	14	128	77	81 duplicate
16077	60 Glycerol-3-phosphate	55 [612; 4-Aminobutyric acid (2TBS)]	0.648	36,027	0.507	12	130	15	127	138	42 duplicate
13627	60 Glycerol-3-phosphate	30 [815; Ethyl-3(2H)-thiophenone]	0.601	11,515	0.426	13	129	18	124	24	103 duplicate
6631	60 Glycerol-3-phosphate	69 Arginine	0.601	11,515	0.426	13	129	18	124	24	103 duplicate
6657	60 Glycerol-3-phosphate	85 [770; 3,4,6-Trisubstituted phenylethanolamine (5TMS)]	0.587	33,328	0.454	15	127	23	119	132	32 original
13946	60 Glycerol-3-phosphate	32 [729; N,N-Dimethyllysine methyl ester]	0.683	27,995	0.495	16	128	10	132	119	50 duplicate
6699	60 Glycerol-3-phosphate	137 Ergosterol	0.568	12,701	0.392	17	125	25	117	29	123 original
15454	60 Glycerol-3-phosphate	48 Asparagine	0.538	19,542	0.510	18	123	28	114	72	39 duplicate

13954	60 Glycerol-3-phosphate	33 Methionine	64	0.423	0.515	18.709	0.406	19	124	31	111	66	116 duplicate
15727	60 Glycerol-3-phosphate	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	0.408	0.567	33.940	0.465	20	122	26	116	134	72 duplicate
13737	60 Glycerol-3-phosphate	31 [622; Parabanic acid (2TMS)]	64	0.399	0.555	26.337	0.438	21	121	27	115	110	88 duplicate
11086	60 Glycerol-3-phosphate	9 Proline	63	0.389	0.679	13.616	0.507	22	120	11	131	33	41 duplicate
8700	60 Glycerol-3-phosphate	138 [674; Ergosterol (1TMS)]	46	0.387	0.585	30.129	0.451	23	119	24	118	123	89 original
6628	60 Glycerol-3-phosphate	66 Glycine acid-3-phosphate	64	0.379	0.663	21.723	0.511	24	118	12	130	84	37 original
14061	60 Glycerol-3-phosphate	34 Aspartic acid	64	0.344	0.480	13.080	0.381	25	117	34	108	30	128 duplicate
6656	60 Glycerol-3-phosphate	94 Hexadecanoic acid	64	0.342	0.470	7.570	0.476	26	116	35	107	6	59 original
6670	60 Glycerol-3-phosphate	108 Octadecanoic acid	64	0.332	0.506	22.260	0.390	27	115	33	109	87	124 original
6686	60 Glycerol-3-phosphate	124 [734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]	59	0.321	0.465	39.744	0.374	28	114	36	106	140	131 original
14272	60 Glycerol-3-phosphate	36 [596; N-Acetylglutamic acid (2TMS)]	64	0.318	0.561	8.730	0.535	29	113	13	129	9	21 duplicate
8703	60 Glycerol-3-phosphate	141 Lanosta-8,24-dien-3-beta-ol	61	0.317	0.450	29.850	0.442	30	112	38	104	122	94 original
6678	60 Glycerol-3-phosphate	116 [882; Pseudouridine (5TMS)]	30	0.310	0.524	18.998	0.456	31	111	30	112	70	80 original
6673	60 Glycerol-3-phosphate	111 [583; Erythritol (4TMS)]	42	0.310	0.347	32.953	0.339	32	110	51	91	131	138 original
10954	60 Glycerol-3-phosphate	8 Isoleucine	55	0.298	0.590	12.603	0.484	33	109	22	120	28	54 duplicate
10141	60 Glycerol-3-phosphate	2 Serine	62	0.298	0.619	14.012	0.503	34	108	17	125	37	44 duplicate
6623	60 Glycerol-3-phosphate	61 [NA]	64	0.292	0.415	18.930	0.416	35	107	41	101	69	110 original
6645	60 Glycerol-3-phosphate	83 Sorbitol	58	0.290	0.595	6.811	0.529	36	106	20	122	3	27 original
6671	60 Glycerol-3-phosphate	109 Octadecanoic acid	64	0.290	0.382	12.226	0.392	37	105	45	97	27	121 original
6693	60 Glycerol-3-phosphate	131 [626; 5-Methylthiadenosine (3TMS)]	55	0.282	0.182	31.472	0.530	38	104	60	82	128	26 original
6698	60 Glycerol-3-phosphate	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.279	0.457	9.924	0.288	39	103	37	105	13	141 original
15816	60 Glycerol-3-phosphate	52 [NA]	46	0.277	0.534	30.914	0.608	40	102	29	113	125	1 duplicate
10552	60 Glycerol-3-phosphate	5 Leucine	45	0.275	0.181	22.707	0.484	41	101	61	81	91	55 duplicate
6681	60 Glycerol-3-phosphate	119 [931; myo-Inositol-2-phosphate (7TMS)]	64	0.270	0.423	17.712	0.444	42	100	39	103	60	93 original
15172	60 Glycerol-3-phosphate	45 Homocysteine	61	0.258	0.265	37.929	0.367	43	99	57	85	139	134 duplicate
6669	60 Glycerol-3-phosphate	107 9-(Z)-Octadecenoic acid	64	0.254	0.393	8.489	0.451	44	98	42	100	7	87 original
6644	60 Glycerol-3-phosphate	82 Lysine	39	0.244	0.366	13.200	0.557	45	97	49	93	32	13 original
12829	60 Glycerol-3-phosphate	23 Homoserine	64	0.237	0.372	18.760	0.495	46	96	48	94	68	49 duplicate
6637	60 Glycerol-3-phosphate	75 Lysine	64	0.228	0.592	19.223	0.503	47	95	21	121	71	45 original
6660	60 Glycerol-3-phosphate	98 [697; Ribose-5-phosphate methoxamine (5TMS)]	48	0.225	0.390	32.385	0.440	48	94	43	99	129	95 original
8702	60 Glycerol-3-phosphate	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49	0.218	0.306	30.867	0.414	49	93	54	88	124	112 original
8701	60 Glycerol-3-phosphate	139 [700; Ergosta-5,7-dien-3-ol]	38	0.201	0.270	31.370	0.424	50	92	58	86	126	105 original
6695	60 Glycerol-3-phosphate	133 [855; Squalene]	64	0.198	0.382	18.611	0.385	51	91	46	96	65	128 original
6651	60 Glycerol-3-phosphate	89 [775; Dopamine (4TMS)]	35	0.193	0.380	25.705	0.498	52	90	47	95	107	48 original
16402	60 Glycerol-3-phosphate	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	0.166	0.514	9.367	0.472	53	89	32	110	10	61 duplicate
12472	60 Glycerol-3-phosphate	20 [619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	0.166	0.328	27.002	0.581	54	88	52	90	113	5 duplicate
15546	60 Glycerol-3-phosphate	49 [877; Pyrophosphoric acid (4TMS)]	64	0.154	0.123	35.566	0.361	55	87	64	78	136	135 duplicate
6647	60 Glycerol-3-phosphate	85 [529; Malic acid (4TMS)]	48	0.147	0.240	18.504	0.462	56	86	58	84	64	76 original
13291	60 Glycerol-3-phosphate	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	0.135	0.323	31.467	0.412	57	85	53	89	127	114 duplicate
6688	60 Glycerol-3-phosphate	126 [559; Erythritol (4TMS)]	45	0.131	0.358	18.452	0.540	58	84	50	92	63	17 original
6692	60 Glycerol-3-phosphate	130 Trehalose	63	0.126	0.235	10.214	0.417	59	83	59	83	17	109 original
13062	60 Glycerol-3-phosphate	25 [709; 2,5-Diaminovalerolactam (2TMS)]	48	0.117	0.296	24.544	0.470	60	82	55	87	102	66 duplicate
6652	60 Glycerol-3-phosphate	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	64	0.089	0.101	17.552	0.434	61	81	66	76	57	98 original
6625	60 Glycerol-3-phosphate	63 Glutamine	52	0.084	0.421	25.290	0.466	62	80	40	102	104	69 original
6676	60 Glycerol-3-phosphate	114 Fructose-6-phosphate	53	0.081	-0.191	23.287	0.554	63	79	85	57	96	15 original
6685	60 Glycerol-3-phosphate	123 [945; Galactofuranose-6-phosphate (7TMS)]	64	0.065	-0.067	13.177	0.540	64	78	72	70	31	16 original
6697	60 Glycerol-3-phosphate	[902; Melibiose (8TMS); alpha-D-Gal(1,6)-D-Glc (8TMS)]	64	0.061	0.123	10.577	0.398	65	77	63	79	20	119 original

6658	60	Glycerol-3-phosphate	96	myo-Inositol	49	0.051	0.108	34,860	0.368	66	76	65	77	135	132 original
6675	60	Glycerol-3-phosphate	113	Galactose-6-phosphate	62	0.043	-0.291	24,058	0.536	67	75	92	50	99	19 original
6638	60	Glycerol-3-phosphate	74	[912; Tetradecanoic acid (1TMS)]	64	0.019	0.143	23,144	0.427	68	74	82	50	99	102 original
6694	60	Glycerol-3-phosphate	132	[895; Isomallose methoxyamine (8TMS)]	42	0.006	-0.262	27,107	0.396	69	73	89	53	114	125 original
14782	60	Glycerol-3-phosphate	41	[639; Proline (2TMS)]	64	0.003	0.004	10,855	0.573	70	72	89	73	22	7 duplicate
6626	60	Glycerol-3-phosphate	4	[789; Tyramine (3TMS)]	63	-0.001	-0.076	20,459	0.335	71	71	75	67	78	140 original
10416	60	Glycerol-3-phosphate	4	Phosphoric acid	51	-0.009	-0.387	13,944	0.468	72	70	44	98	36	70 duplicate
15078	60	Glycerol-3-phosphate	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	-0.014	0.059	16,391	0.505	73	69	67	75	47	43 duplicate
12351	60	Glycerol-3-phosphate	19	Alanine (BP) (3TMS)	64	-0.030	-0.152	13,931	0.607	74	68	80	62	35	2 duplicate
12229	60	Glycerol-3-phosphate	18	[548; Leucine (2TBS)]	64	-0.034	0.025	16,517	0.368	75	67	68	74	48	133 duplicate
14979	60	Glycerol-3-phosphate	43	[500; 1-Acetyl-2-thiohydantoin]	60	-0.034	-0.059	17,399	0.458	76	66	70	72	55	79 duplicate
6664	60	Glycerol-3-phosphate	102	[904; Galactose methoxyamine (5TMS)]	64	-0.036	-0.067	22,332	0.409	77	65	71	71	89	115 original
6680	60	Glycerol-3-phosphate	118	[928; Glucopyranose-6-phosphate (6TMS)]	58	-0.053	-0.183	22,801	0.375	78	64	84	58	92	130 original
6674	60	Glycerol-3-phosphate	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	-0.053	-0.087	33,563	0.452	79	63	73	69	133	85 original
11857	60	Glycerol-3-phosphate	15	Alanine	64	-0.063	-0.247	10,033	0.478	80	62	87	55	15	57 duplicate
6634	60	Glycerol-3-phosphate	72	[918; D-Xylopyranose (4TMS)]	63	-0.071	-0.118	23,772	0.340	81	61	77	65	98	137 original
6689	60	Glycerol-3-phosphate	127	[777; Fructose-6-phosphate methoxyamine (8TMS)]	39	-0.072	-0.074	14,613	0.353	82	60	74	68	42	136 original
6666	60	Glycerol-3-phosphate	104	[795; Erythritol (4TMS)]	63	-0.080	-0.131	20,154	0.512	83	59	78	64	75	38 original
6662	60	Glycerol-3-phosphate	100	[657; Mannitol (6TMS)]	64	-0.083	-0.181	15,267	0.376	84	58	83	59	45	129 original
6646	60	Glycerol-3-phosphate	84	Mannitol	62	-0.094	-0.603	17,359	0.559	85	57	121	21	54	12 original
6684	60	Glycerol-3-phosphate	122	[644; Erythritol (4TMS)]	52	-0.107	-0.383	28,969	0.472	86	58	79	63	121	62 original
6641	60	Glycerol-3-phosphate	79	Glucose	54	-0.119	-0.166	24,187	0.570	87	55	101	41	53	11 original
6672	60	Glycerol-3-phosphate	110	[715; Erythritol (4TMS)]	55	-0.126	-0.091	28,708	0.429	88	54	82	60	100	8 original
6683	60	Glycerol-3-phosphate	121	[657; Erythritol (4TMS)]	62	-0.155	-0.382	10,205	0.461	90	52	100	42	16	77 original
6677	60	Glycerol-3-phosphate	115	Glucose-6-phosphate	60	-0.157	-0.408	32,729	0.484	91	51	104	38	130	73 original
6655	60	Glycerol-3-phosphate	93	[607; Putrescine (4TMS)]	56	-0.160	-0.161	21,395	0.433	92	50	81	61	82	99 original
6679	60	Glycerol-3-phosphate	117	[724; Glycerol (3TMS)]	64	-0.168	-0.241	7,148	0.432	93	49	86	56	4	100 duplicate
13177	60	Glycerol-3-phosphate	26	Citramalic acid	64	-0.189	-0.459	21,935	0.462	94	48	107	35	85	75 duplicate
14167	60	Glycerol-3-phosphate	35	Pyroglutamic acid	64	-0.209	-0.252	14,139	0.404	95	47	88	54	39	117 original
6690	60	Glycerol-3-phosphate	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	57	-0.209	-0.271	24,664	0.394	96	46	90	52	103	127 original
6635	60	Glycerol-3-phosphate	73	[708; Glucose methoxyamine (5TMS)]	64	-0.228	-0.297	8,540	0.416	98	44	83	49	8	111 duplicate
14682	60	Glycerol-3-phosphate	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.211	-0.287	14,631	0.447	97	45	91	51	43	90 duplicate
12592	60	Glycerol-3-phosphate	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	-0.231	-0.377	14,766	0.455	99	43	99	43	44	82 duplicate
13404	60	Glycerol-3-phosphate	28	Malic acid	63	-0.236	-0.403	27,836	0.420	100	42	103	39	118	107 duplicate
11476	60	Glycerol-3-phosphate	12	Glyceric acid	52	-0.240	-0.368	27,365	0.419	101	41	97	45	115	108 duplicate
12711	60	Glycerol-3-phosphate	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	-0.242	-0.370	27,635	0.395	103	40	98	44	117	120 duplicate
15904	60	Glycerol-3-phosphate	53	Glycerol-2-phosphate	64	-0.261	-0.492	14,398	0.467	104	38	109	33	40	68 original
6638	60	Glycerol-3-phosphate	76	Fructose	54	-0.279	-0.313	11,251	0.424	105	37	94	48	23	104 original
6682	60	Glycerol-3-phosphate	120	[945; Uridine (3TMS)]	62	-0.289	-0.417	26,012	0.445	106	36	105	37	109	92 original
6640	60	Glycerol-3-phosphate	78	Mannose	64	-0.291	-0.439	25,833	0.445	107	35	106	36	108	91 duplicate
11731	60	Glycerol-3-phosphate	14	Fumaric acid	62	-0.292	-0.387	19,748	0.561	108	34	102	40	73	10 original
6688	60	Glycerol-3-phosphate	106	[733; Threitol (4TMS)]	64	-0.312	-0.566	16,998	0.472	109	33	114	28	52	63 original
6687	60	Glycerol-3-phosphate	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	70	-0.313	-0.364	9,935	0.392	110	32	96	46	14	122 original
8632	60	Glycerol-3-phosphate	6	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	64	-0.323	-0.571	22,307	0.475	111	31	117	25	88	60 duplicate
10687	60	Glycerol-3-phosphate	11	Glycerol	64	-0.344	-0.483	16,895	0.420	112	30	108	34	50	106 duplicate
11347	60	Glycerol-3-phosphate	105	[705; 2-Ketogluconic acid (5TMS)]	48	-0.362	-0.544	16,831	0.494	113	29	112	30	49	51 original
6667	60	Glycerol-3-phosphate	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.367	-0.505	17,671	0.437	114	28	110	32	59	97 duplicate
14479	60	Glycerol-3-phosphate	54	[NA]	55	-0.385	-0.559	26,484	0.470	115	27	113	29	111	65 duplicate
15991	60	Glycerol-3-phosphate	92	[680; Glycerol-2-phosphate (4TMS)]	54	-0.389	-0.623	20,369	0.403	116	26	111	31	76	118 original
6654	60	Glycerol-3-phosphate	80	[772; D-Glucose (5TMS)]	62	-0.395	-0.600	16,941	0.413	117	25	120	22	51	113 original

13516	60 Glycerol-3-phosphate	29 Erythritol	64 -0.387	-0.588	20.597	0.466	118	24	118	28	79	71 duplicate
6624	60 Glycerol-3-phosphate	32 [812; D-Xylofuranose (4TMS)]	64 -0.431	-0.583	10.552	0.468	119	23	118	24	19	67 original
14581	60 Glycerol-3-phosphate	39 [826; 1-Phenylethanol (1TMS)]	64 -0.436	-0.566	18.346	0.451	120	22	115	27	62	88 duplicate
6661	60 Glycerol-3-phosphate	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41 -0.446	-0.595	22.812	0.492	121	21	119	23	93	52 original
15361	60 Glycerol-3-phosphate	47 [NA]	64 -0.448	-0.607	22.378	0.471	122	20	123	19	90	64 duplicate
6648	60 Glycerol-3-phosphate	86 [793; D-Galactono-1,4-lactone (4TMS)]	61 -0.450	-0.616	23.057	0.508	123	19	125	17	94	40 original
11982	60 Glycerol-3-phosphate	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	64 -0.461	-0.628	10.852	0.539	124	18	128	14	21	18 duplicate
6650	60 Glycerol-3-phosphate	88 Gluconic acid	64 -0.466	-0.611	18.069	0.536	125	16	124	18	61	20 original
12108	60 Glycerol-3-phosphate	17 [700; 2-methyl-1,2-propanediol (2TMS)]	64 -0.468	-0.619	12.163	0.451	126	17	126	16	26	88 duplicate
12846	60 Glycerol-3-phosphate	24 [725; 2-Ketooctanoic acid (2TMS)]	64 -0.469	-0.636	15.414	0.531	127	15	130	12	46	25 duplicate
16235	60 Glycerol-3-phosphate	56 [829; Orolic acid (3TMS)]	64 -0.474	-0.651	26.538	0.519	128	14	132	10	112	30 duplicate
6649	60 Glycerol-3-phosphate	87 [945; beta-D-Glucofuranose (5TMS)]	62 -0.475	-0.633	20.087	0.491	129	13	129	13	74	53 original
16319	60 Glycerol-3-phosphate	57 [757; 2-Desoxy-pentose-3-ylose dimethoxyamine (2TMS)]	55 -0.481	-0.605	20.600	0.478	130	12	122	20	80	58 duplicate
6665	60 Glycerol-3-phosphate	103 [648; Ethylamine (2TMS)]	63 -0.483	-0.703	22.135	0.500	131	11	137	5	86	47 original
15267	60 Glycerol-3-phosphate	46 Arabinose	64 -0.514	-0.654	21.203	0.511	132	10	135	7	81	38 duplicate
6627	60 Glycerol-3-phosphate	65 [646; 3-Deoxyglucitol (5TMS)]	63 -0.515	-0.620	27.593	0.513	133	9	127	15	116	35 original
6659	60 Glycerol-3-phosphate	97 [756; beta-D-Methylglucopyranoside (4TMS)]	52 -0.516	-0.795	16.757	0.579	134	8	141	1	67	6 original
11604	60 Glycerol-3-phosphate	13 Ureacil	64 -0.517	-0.652	14.031	0.529	135	6	133	9	38	28 duplicate
6663	60 Glycerol-3-phosphate	101 [832; Dopamine (4TMS)]	64 -0.517	-0.754	21.468	0.480	136	7	139	3	83	56 original
15637	60 Glycerol-3-phosphate	50 [746; Ribonic acid-1,4-lactone (3TMS)]	61 -0.519	-0.658	35.654	0.455	137	5	136	6	137	83 duplicate
6653	60 Glycerol-3-phosphate	91 [766; beta-D-Methylglucopyranoside (4TMS)]	64 -0.523	-0.779	25.529	0.514	138	4	140	2	105	33 original
6696	60 Glycerol-3-phosphate	134 Isomaltose	64 -0.541	-0.649	17.551	0.513	139	3	131	11	56	34 original
6691	60 Glycerol-3-phosphate	128 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59 -0.546	-0.652	23.530	0.532	140	2	134	8	97	24 original
10002	60 Glycerol-3-phosphate	1 [938; Sulfuric acid (2TMS)]	36 -0.549	-0.734	17.629	0.534	141	1	138	4	58	22 duplicate
6710	61 [NA]	68 [570; Hypoxanthine (2TMS)]	20.684	0.825	14.258	0.442	1	141	1	141	70	65 original
10553	61 [NA]	5 Leucine	45 0.628	0.457	8.704	0.348	2	140	18	124	24	124 duplicate
15728	61 [NA]	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44 0.628	0.664	18.725	0.516	3	139	6	136	104	9 duplicate
16078	61 [NA]	55 [612; 4-Aminobutyric acid (2TBS)]	43 0.604	0.717	20.366	0.491	4	138	4	138	111	30 duplicate
6724	61 [NA]	82 Lysine	39 0.592	0.649	13.815	0.519	5	137	7	135	64	4 original
6731	61 [NA]	89 [775; Dopamine (4TMS)]	35 0.566	0.756	14.465	0.503	6	136	2	140	71	18 original
6705	61 [NA]	63 Glutamine	52 0.534	0.731	13.135	0.505	7	135	3	139	59	16 original
13628	61 [NA]	30 [815; Ethyl-3(2H)-thiophenone]	64 0.498	0.425	27.417	0.365	8	134	22	120	125	118 duplicate
15455	61 [NA]	48 Asparagine	64 0.494	0.643	8.681	0.531	9	133	8	134	23	1 duplicate
13955	61 [NA]	33 Methionine	64 0.484	0.434	8.561	0.390	10	132	20	122	21	101 duplicate
15817	61 [NA]	52 [NA]	46 0.474	0.689	17.940	0.526	11	131	5	137	96	2 duplicate
6719	61 [NA]	77 [826; beta-[[[5-methyl-2-thienyl)methyl]amino]-benzeneacetic acid methyl ester]	62 0.458	0.451	27.227	0.403	12	130	19	123	123	90 original
15173	61 [NA]	45 Homocysteine	61 0.457	0.509	20.141	0.384	13	129	15	127	109	102 duplicate
6723	61 [NA]	81 Tyrosine	64 0.455	0.525	31.521	0.499	14	127	13	129	134	22 original
14377	61 [NA]	37 Phenylalanine	64 0.455	0.508	20.268	0.423	15	128	16	128	110	78 duplicate
6737	61 [NA]	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50 0.451	0.519	18.254	0.427	16	126	14	128	99	72 original
11218	61 [NA]	10 Glycine	64 0.450	0.561	16.098	0.516	17	125	9	133	84	8 duplicate
6773	61 [NA]	131 [626; 5-Methylthiodenosine (3TMS)]	55 0.445	0.496	14.734	0.464	18	124	17	125	75	31 original
14882	61 [NA]	42 Glutamic acid	60 0.427	0.294	27.348	0.392	19	123	34	108	124	96 duplicate
6711	61 [NA]	69 Arginine	60 0.426	0.420	18.579	0.468	20	122	24	118	103	44 original
6709	61 [NA]	67 Citric acid	64 0.425	0.547	21.385	0.454	21	121	10	132	112	55 original
10280	61 [NA]	3 Ethanolamine	62 0.415	0.540	9.261	0.512	22	120	11	131	29	14 duplicate
14062	61 [NA]	34 Aspartic acid	64 0.408	0.425	30.434	0.391	23	119	23	119	130	98 duplicate

12473	61 [NA]	20 [619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31 0,402	0,537	14,141	0,513	24 118	12 130	68	13 duplicate
16485	61 [NA]	59 Ornithine; Arginine	64 0,397	0,431	38,732	0,384	25 117	21 121	139	104 duplicate
10955	61 [NA]	8 Isoleucine	55 0,380	0,138	16,890	0,302	26 116	46 98	89	138 duplicate
15547	61 [NA]	49 [877; Pyrophosphoric acid (4TMS)]	64 0,374	0,415	18,478	0,415	27 115	25 117	102	84 duplicate
12830	61 [NA]	23 Homoserine	64 0,344	0,391	8,593	0,405	28 114	27 115	22	89 duplicate
11087	61 [NA]	9 Proline	63 0,314	0,224	25,589	0,344	29 113	39 103	121	126 duplicate
13738	61 [NA]	31 [622; Parabenic acid (2TMS)]	64 0,312	0,354	9,084	0,377	30 112	28 114	28	108 duplicate
13847	61 [NA]	32 [729; N,N-Dimethyllysine methyl ester]	63 0,304	0,327	14,578	0,414	31 111	28 113	72	85 duplicate
6740	61 [NA]	98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	48 0,300	0,326	17,723	0,370	32 110	30 112	95	114 original
16586	61 [NA]	60 Glycerol-3-phosphate	64 0,292	0,415	18,930	0,416	33 109	28 116	105	83 duplicate
10822	61 [NA]	7 Threonine	64 0,285	0,321	27,931	0,361	34 108	31 111	127	121 duplicate
6750	61 [NA]	108 Octadecenoic acid	64 0,283	0,285	6,001	0,384	35 107	35 107	9	103 original
13063	61 [NA]	25 [709; 2,5-Diaminovalerolactam (2TMS)]	48 0,257	0,200	13,574	0,436	36 106	41 101	61	69 duplicate
6708	61 [NA]	66 Glycemic acid-3-phosphate	64 0,222	0,254	5,163	0,346	37 105	37 105	4	125 original
6749	61 [NA]	107 9-(Z)-Octadecenoic acid	64 0,194	0,298	11,906	0,369	38 104	32 110	47	115 original
6735	61 [NA]	93 [607; Putrescine (4TMS)]	60 0,193	0,157	15,550	0,392	39 103	42 100	77	97 original
10142	61 [NA]	2 Serine	62 0,184	0,131	17,280	0,368	40 102	47 95	92	116 duplicate
6732	61 [NA]	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	64 0,177	0,213	5,286	0,364	41 101	40 102	5	119 original
14980	61 [NA]	43 [548; Leucine (2TMS)]	60 0,178	0,143	6,003	0,391	42 100	44 98	10	98 duplicate
6726	61 [NA]	84 Mannitol	62 0,166	0,062	29,807	0,393	43 99	54 88	128	95 original
10003	61 [NA]	1 [938; Sulfuric acid (2TMS)]	36 0,165	-0,050	8,084	0,426	44 98	63 79	18	74 duplicate
6713	61 [NA]	71 [731; Erythrose (3TMS)]	64 0,154	0,253	9,331	0,373	45 97	38 104	30	112 original
6761	61 [NA]	119 [831; myo-Inositol-2-phosphate (7TMS)]	64 0,151	0,294	6,289	0,402	46 96	33 109	11	92 original
13282	61 [NA]	27 [815; (E)-4-Methyl-5-hydroxy-3-pentan-2-one (1TMS)]	53 0,134	0,261	17,523	0,380	47 95	36 108	94	106 duplicate
6717	61 [NA]	75 Lysine	64 0,101	0,123	37,639	0,339	48 94	48 94	138	128 original
6779	61 [NA]	137 Ergosterol	64 0,064	0,151	12,503	0,331	49 93	43 99	54	132 original
15905	61 [NA]	53 Glycerol-2-phosphate	64 0,063	-0,020	9,746	0,321	50 92	61 81	34	135 duplicate
6753	61 [NA]	111 [563; Erythritol (4TMS)]	42 0,057	0,141	18,100	0,419	51 91	45 97	97	80 original
6781	61 [NA]	139 [700; Ergosta-5,7-dien-3-ol]	38 0,053	0,108	16,794	0,342	52 90	49 93	88	127 original
14273	61 [NA]	36 [596; N-Acetylglutamic acid (2TMS)]	64 0,053	0,078	26,575	0,339	53 89	50 92	122	129 duplicate
6768	61 [NA]	124 [734; 1-Monoolcylglycerol (2TMS); 1-Monohexadecenylglycerol (1TMS)]	59 0,039	-0,005	22,256	0,362	54 88	58 84	115	120 original
6706	61 [NA]	64 [789; Tyramine (3TMS)]	63 0,028	-0,034	4,523	0,399	55 87	62 80	3	94 original
6772	61 [NA]	130 Trehalose	63 0,012	-0,094	27,874	0,351	56 86	67 75	126	122 original
6741	61 [NA]	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41 0,000	-0,424	10,772	0,475	57 85	105 37	42	36 original
6783	61 [NA]	141 Lanosta-8,24-dien-3-beta-ol	61 -0,033	0,060	13,003	0,326	58 84	55 87	58	133 original
10417	61 [NA]	4 Phosphoric acid	51 -0,034	-0,072	31,263	0,261	59 83	65 77	133	141 duplicate
16403	61 [NA]	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64 -0,035	0,070	14,075	0,349	60 82	52 90	66	123 duplicate
6777	61 [NA]	[902; Melibiose (8TMS); alpha-D-Gal(1,6)-D-Glc (8TMS)]	64 -0,051	0,069	9,553	0,371	61 81	53 89	33	113 original
6736	61 [NA]	94 Hexadecanoic acid	64 -0,072	-0,184	20,108	0,360	62 80	71 71	108	105 original
6747	61 [NA]	105 [705; 2-Ketogluconic acid (5TMS)]	48 -0,073	0,040	12,434	0,449	63 79	56 88	52	61 original
6751	61 [NA]	109 Octadecenoic acid	64 -0,075	-0,256	21,630	0,414	64 78	80 62	114	88 original
6775	61 [NA]	133 [855; Squalene]	64 -0,077	-0,084	7,349	0,337	65 77	66 76	16	130 original
6778	61 [NA]	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17 -0,088	-0,283	3,412	0,443	66 76	83 59	1	63 original
6758	61 [NA]	116 [882; Pseudouridine (5TMS)]	30 -0,090	-0,014	8,928	0,303	67 75	59 83	27	137 original
6714	61 [NA]	72 [919; D-Xylopyranose (4TMS)]	63 -0,097	-0,238	9,495	0,314	68 74	78 64	32	136 original
6780	61 [NA]	138 [674; Ergosterol (1TMS)]	46 -0,100	-0,159	15,147	0,367	69 73	69 73	76	117 original
6782	61 [NA]	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49 -0,100	-0,018	14,634	0,333	70 72	60 82	73	131 original

15992	61 [NA]	54 [NA]	55 -0.102	-0.164	12.075	0.441	71	71	70	72	49	67 duplicate
6725	61 [NA]	83 Sorbitol	58 -0.112	0.032	18.951	0.288	72	70	57	85	108	140 original
16320	61 [NA]	57 [757; 2-Desoxy-pentose dimethoxyamine (2TMS)]	55 -0.115	-0.394	15.778	0.455	73	69	100	42	82	53 duplicate
6739	61 [NA]	97 [756; beta-D-Methylglucopyranoside (4TMS)]	52 -0.127	-0.291	21.561	0.467	74	68	87	55	113	45 original
6744	61 [NA]	102 [904; Galactose methoxyamine (5TMS)]	64 -0.129	0.074	5.544	0.409	75	67	51	91	8	88 original
6738	61 [NA]	98 myo-Inositol	49 -0.141	-0.146	18.430	0.294	76	66	68	74	101	139 original
6770	61 [NA]	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45 -0.141	-0.205	8.512	0.474	77	65	75	67	20	38 original
6754	61 [NA]	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63 -0.148	-0.198	15.590	0.422	78	64	74	68	78	78 original
6727	61 [NA]	85 [529; Methylcitric acid (4TMS)]	48 -0.149	-0.187	4.346	0.321	79	63	72	70	2	134 original
11858	61 [NA]	15 Alanine	64 -0.152	-0.446	17.220	0.491	80	62	108	34	91	28 duplicate
6769	61 [NA]	127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	39 -0.162	-0.233	5.458	0.454	81	61	77	65	7	58 original
6734	61 [NA]	92 [680; Glycerol-2-phosphate (4TMS)]	54 -0.163	-0.507	10.487	0.463	82	60	118	24	40	49 original
11477	61 [NA]	12 Glycemic acid	63 -0.169	-0.230	10.461	0.390	83	59	76	66	39	100 duplicate
15362	61 [NA]	47 [NA]	64 -0.204	-0.339	11.664	0.375	84	58	91	51	48	109 duplicate
6742	61 [NA]	100 [857; Mannitol (6TMS)]	64 -0.210	-0.051	6.832	0.416	85	57	64	78	14	82 original
13517	61 [NA]	29 Erythritol	64 -0.228	-0.292	5.342	0.424	86	56	88	54	6	75 duplicate
6716	61 [NA]	74 [912; Tetradecanoic acid (1TMS)]	64 -0.231	-0.288	11.480	0.379	87	55	85	57	44	107 original
12230	61 [NA]	18 [590; 1-Acetyl-2-thiohydantoin]	64 -0.236	-0.245	6.424	0.374	88	54	79	63	12	110 duplicate
6733	61 [NA]	91 [766; beta-D-Methylglucopyranoside (4TMS)]	64 -0.243	-0.275	18.416	0.400	89	53	82	60	100	93 original
11348	61 [NA]	11 Succinic acid	64 -0.249	-0.291	6.568	0.468	91	51	86	56	13	43 duplicate
6774	61 [NA]	132 [895; Isomaltose methoxyamine (8TMS)]	42 -0.259	-0.527	15.707	0.454	92	50	124	18	81	54 original
11893	61 [NA]	16 [844; 2-Methyl-1,3-butanediol (2TMS)]	64 -0.265	-0.392	16.528	0.483	93	49	99	43	88	33 duplicate
12947	61 [NA]	24 [725; 2-Ketocotanoic acid (2TMS)]	64 -0.269	-0.446	30.713	0.500	94	48	109	33	131	18 duplicate
12107	61 [NA]	17 [700; 2-methyl-1,2-propanediol (2TMS)]	64 -0.270	-0.399	16.711	0.467	95	48	101	41	87	48 duplicate
16236	61 [NA]	56 [828; Oroic acid (3TMS)]	64 -0.270	-0.494	13.804	0.489	96	47	116	26	63	20 duplicate
13405	61 [NA]	28 Malic acid	64 -0.273	-0.341	7.613	0.450	97	45	92	50	17	59 duplicate
12593	61 [NA]	21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64 -0.274	-0.286	14.670	0.411	98	44	84	58	74	87 duplicate
15077	61 [NA]	44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	50 -0.275	-0.197	10.845	0.454	99	43	73	69	43	56 duplicate
6771	61 [NA]	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59 -0.279	-0.485	14.207	0.518	100	42	115	27	69	5 original
6707	61 [NA]	65 [646; 3-Deoxyglucitol (5TMS)]	63 -0.283	-0.460	16.438	0.508	101	41	113	28	85	15 original
12712	61 [NA]	22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52 -0.284	-0.457	12.561	0.494	102	40	111	31	56	26 duplicate
6721	61 [NA]	79 Glucose	64 -0.286	-0.583	33.598	0.473	103	39	128	13	136	39 original
6767	61 [NA]	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64 -0.288	-0.601	31.075	0.489	104	38	132	10	132	23 original
6762	61 [NA]	120 [945; Uridine (3TMS)]	54 -0.289	-0.262	10.227	0.472	105	37	81	37	40	37 original
6755	61 [NA]	113 Galactose-6-phosphate	62 -0.293	-0.596	10.272	0.514	106	36	130	12	38	10 original
14582	61 [NA]	39 [829; 1-Phenylethanol (1TMS)]	63 -0.294	-0.405	17.097	0.454	107	35	103	39	90	57 duplicate
6743	61 [NA]	101 [832; Dopamine (4TMS)]	64 -0.299	-0.332	11.916	0.403	108	34	90	52	48	91 original
14480	61 [NA]	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	64 -0.302	-0.366	7.343	0.459	109	33	94	48	15	51 duplicate
6776	61 [NA]	134 Isomaltose	64 -0.305	-0.508	25.197	0.513	110	32	119	23	120	12 original
6704	61 [NA]	62 [812; D-Xylofuranose (4TMS)]	64 -0.306	-0.441	12.321	0.483	111	31	107	35	50	32 original
11732	61 [NA]	14 Fumaric acid	64 -0.307	-0.376	8.796	0.423	112	30	96	46	25	77 duplicate
6768	61 [NA]	126 [559; Erythritol (4TMS)]	45 -0.309	-0.412	8.215	0.498	113	29	104	38	19	24 original
15288	61 [NA]	46 Arabinose	64 -0.310	-0.527	19.211	0.517	114	28	123	19	107	6 duplicate
13745	61 [NA]	103 [648; Ethylamine (2TMS)]	63 -0.312	-0.345	15.645	0.431	115	27	93	49	79	71 original
6718	61 [NA]	28 Citramalic acid	64 -0.318	-0.388	14.077	0.442	116	26	97	45	67	66 duplicate
6730	61 [NA]	88 Gluconic acid	64 -0.323	-0.460	12.830	0.474	117	25	114	28	57	37 original
6756	61 [NA]	114 Fructose-6-phosphate	53 -0.324	-0.564	9.872	0.505	118	24	128	14	35	17 original
6760	61 [NA]	118 [928; Glucopyranose-6-phosphate (6TMS)]	58 -0.325	-0.623	10.127	0.465	119	23	136	6	36	47 original
15638	61 [NA]	50 [746; Ribonic acid-1,4-lactone (3TMS)]	61 -0.331	-0.435	16.246	0.421	120	22	106	36	98	79 duplicate

10688	61 [NA]	6	Glycerol	64	-0.341	-0.597	40.063	0.478	121	21	131	11	141	35 duplicate
11605	61 [NA]	13	Uracil	64	-0.342	-0.458	15.902	0.472	122	20	112	30	83	41 duplicate
6728	61 [NA]	86	[793; D-Galactono-1,4-lactone (4TMS)]	61	-0.343	-0.554	23.636	0.520	123	19	127	15	117	3 original
6765	61 [NA]	123	[945; Galactofuranose-6-phosphate (7TMS)]	64	-0.357	-0.547	9.491	0.462	124	18	126	16	31	50 original
14168	61 [NA]	35	Pyroglutamic acid	64	-0.358	-0.525	39.619	0.514	125	17	122	20	140	11 duplicate
6715	61 [NA]	73	[708; Glucose methoxyamine (5TMS)]	57	-0.361	-0.452	12.331	0.426	126	16	110	32	51	73 original
14683	61 [NA]	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.362	-0.391	32.498	0.418	127	15	98	44	135	81 duplicate
6764	61 [NA]	122	[644; Erythritol (4TMS)]	52	-0.367	-0.371	15.647	0.434	128	14	95	47	80	70 original
6757	61 [NA]	115	Glucose-6-phosphate	62	-0.377	-0.627	23.254	0.494	129	13	137	5	118	27 original
6746	61 [NA]	104	[795; Erythritol (4TMS)]	63	-0.385	-0.525	8.855	0.439	130	12	121	21	26	68 original
6752	61 [NA]	110	[715; Erythritol (4TMS)]	54	-0.412	-0.495	13.635	0.455	131	11	117	25	62	52 original
6763	61 [NA]	121	[657; Erythritol (4TMS)]	55	-0.418	-0.400	13.904	0.448	132	10	102	40	65	62 original
6720	61 [NA]	78	Mannose	62	-0.420	-0.530	13.176	0.463	133	9	125	17	60	48 original
6718	61 [NA]	76	Fructose	64	-0.434	-0.608	25.132	0.497	134	8	133	9	119	25 original
6712	61 [NA]	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	-0.444	-0.512	17.292	0.449	135	7	120	22	93	60 original
12352	61 [NA]	19	Alanine (BP) (3TMS)	64	-0.454	-0.640	11.660	0.482	136	6	138	4	45	34 duplicate
6759	61 [NA]	117	[724; Glycerol (3TMS)]	56	-0.482	-0.615	10.518	0.442	137	5	135	7	41	64 original
14783	61 [NA]	41	[639; Proline (2TMS)]	64	-0.483	-0.613	12.502	0.471	138	4	134	8	53	42 duplicate
6748	61 [NA]	106	[733; Threitol (4TMS)]	62	-0.510	-0.688	12.546	0.517	139	3	139	3	55	7 original
6729	61 [NA]	87	[945; beta-D-Glucopyranose (5TMS)]	62	-0.520	-0.767	34.539	0.499	140	2	140	2	137	21 original
6722	61 [NA]	80	[772; D-Glucose (5TMS)]	62	-0.542	-0.770	30.042	0.492	141	1	141	1	129	28 original
6807	62 [812; D-Xylofuranose (4'	86	[793; D-Galactono-1,4-lactone (4TMS)]	61	0.766	0.949	15.602	0.669	1	141	1	141	71	4 original
15993	62 [812; D-Xylofuranose (4'	54	[NA]	55	0.752	0.917	18.192	0.611	2	140	9	133	83	29 duplicate
6855	62 [812; D-Xylofuranose (4'	134	Isomaltose	64	0.737	0.939	13.835	0.662	3	139	3	139	56	7 original
12948	62 [812; D-Xylofuranose (4'	24	[725; 2-Ketooctanoic acid (2TMS)]	64	0.733	0.917	18.958	0.652	4	137	8	134	91	10 duplicate
11984	62 [812; D-Xylofuranose (4'	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	0.733	0.897	4.992	0.662	5	138	12	130	5	8 duplicate
16237	62 [812; D-Xylofuranose (4'	56	[829; Oroic acid (3TMS)]	64	0.732	0.935	16.522	0.655	6	136	5	137	77	9 duplicate
6786	62 [812; D-Xylofuranose (4'	55	[646; 3-Deoxyglucitol (5TMS)]	63	0.729	0.935	17.669	0.676	7	135	6	136	86	1 original
15269	62 [812; D-Xylofuranose (4'	46	Arabinose	64	0.728	0.936	12.244	0.669	8	134	4	138	45	3 duplicate
16321	62 [812; D-Xylofuranose (4'	57	[757; 2-Deoxy-pentos-3-yose dimethoxyamine (2TMS)]	55	0.720	0.941	12.761	0.669	9	133	2	140	48	5 duplicate
11349	62 [812; D-Xylofuranose (4'	11	Succinic acid	64	0.711	0.877	7.873	0.611	10	132	20	122	18	28 duplicate
6850	62 [812; D-Xylofuranose (4'	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	0.702	0.929	14.295	0.631	11	131	7	135	59	17 original
11606	62 [812; D-Xylofuranose (4'	13	Uracil	64	0.701	0.898	5.897	0.636	12	130	11	131	12	15 duplicate
6809	62 [812; D-Xylofuranose (4'	88	Gluconic acid	64	0.698	0.870	8.353	0.622	13	129	21	121	19	21 original
14583	62 [812; D-Xylofuranose (4'	39	[829; 1-Phenylethanol (1TMS)]	63	0.697	0.895	9.891	0.621	14	128	13	129	25	22 duplicate
13518	62 [812; D-Xylofuranose (4'	29	Erythritol	64	0.688	0.877	11.929	0.607	15	127	19	123	39	32 duplicate
15639	62 [812; D-Xylofuranose (4'	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	0.684	0.880	27.426	0.585	16	126	18	124	131	45 duplicate
11733	62 [812; D-Xylofuranose (4'	14	Fumaric acid	64	0.676	0.885	17.259	0.585	17	125	16	126	83	30 duplicate
13406	62 [812; D-Xylofuranose (4'	28	Malic acid	64	0.674	0.885	5.819	0.625	18	124	17	125	9	20 duplicate
14481	62 [812; D-Xylofuranose (4'	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.669	0.893	8.366	0.645	19	123	15	127	20	13 duplicate
6846	62 [812; D-Xylofuranose (4'	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	0.663	0.868	18.107	0.589	20	122	23	119	92	44 original
12108	62 [812; D-Xylofuranose (4'	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	0.661	0.861	5.826	0.552	21	121	24	118	10	59 duplicate
14169	62 [812; D-Xylofuranose (4'	35	Pyroglutamic acid	64	0.632	0.903	28.321	0.599	22	120	10	132	134	37 duplicate
12713	62 [812; D-Xylofuranose (4'	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.623	0.831	19.633	0.607	23	119	29	113	95	31 duplicate
6791	62 [812; D-Xylofuranose (4'	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	0.620	0.848	7.464	0.471	24	118	55	87	16	92 original
12594	62 [812; D-Xylofuranose (4'	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	0.615	0.781	3.759	0.544	25	117	35	107	2	61 duplicate
6799	62 [812; D-Xylofuranose (4'	76	Mannose	62	0.615	0.848	16.706	0.557	26	116	28	116	79	57 original
6797	62 [812; D-Xylofuranose (4'	76	Fructose	64	0.614	0.894	13.223	0.599	27	115	14	128	51	38 original
6836	62 [812; D-Xylofuranose (4'	115	Glucose-6-phosphate	62	0.611	0.868	11.689	0.603	28	114	22	120	34	38 original



6827	62 [812; D-Xylofuranose (4' 106 [733; Threitol (4TMS)]	0.807	0.841	10.619	0.651	28	113	27	115	27	11	original
14894	62 [812; D-Xylofuranose (4' 40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	0.604	0.815	21.643	0.597	30	112	30	112	105	41	duplicate
6794	62 [812; D-Xylofuranose (4' 73 [708; Glucose methoxyamine (5TMS)]	0.803	0.796	15.289	0.495	31	111	31	111	67	82	original
6813	62 [812; D-Xylofuranose (4' 92 [680; Glycerol-2-phosphate (4TMS)]	0.600	0.791	13.515	0.583	32	110	32	110	54	47	original
11478	62 [812; D-Xylofuranose (4' 12 Glyceral acid	0.592	0.779	19.493	0.570	33	109	37	105	94	54	duplicate
6824	62 [812; D-Xylofuranose (4' 103 [648; Ethylamine (2TMS)]	0.548	0.741	12.985	0.513	34	108	42	100	50	73	original
6841	62 [812; D-Xylofuranose (4' 120 [945; Uridine (3TMS)]	0.536	0.351	5.536	0.598	35	107	72	70	8	40	original
6823	62 [812; D-Xylofuranose (4' 102 [904; Galactose methoxyamine (5TMS)]	0.533	0.744	3.791	0.539	37	105	41	101	3	65	duplicate
13179	62 [812; D-Xylofuranose (4' 26 Citramalic acid	0.515	0.851	21.814	0.615	39	103	25	117	107	25	original
6853	62 [812; D-Xylofuranose (4' 132 [895; Isomaltose methoxyamine (8TMS)]	0.512	0.839	17.016	0.616	40	102	28	114	82	24	original
6820	62 [812; D-Xylofuranose (4' 89 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	0.508	0.701	6.858	0.537	41	101	47	95	14	68	original
6821	62 [812; D-Xylofuranose (4' 100 [657; Mannitol (6TMS)]	0.508	0.687	25.661	0.525	42	100	51	91	124	71	original
6833	62 [812; D-Xylofuranose (4' 112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	0.508	0.736	14.198	0.571	43	99	44	98	58	52	original
6838	62 [812; D-Xylofuranose (4' 117 [724; Glycerol (3TMS)]	0.482	0.704	22.074	0.590	44	98	46	96	108	43	original
6842	62 [812; D-Xylofuranose (4' 121 [657; Erythritol (4TMS)]	0.481	0.707	12.095	0.473	45	97	57	85	43	90	original
6822	62 [812; D-Xylofuranose (4' 101 [632; Dopamine (4TMS)]	0.457	0.614	9.203	0.502	46	96	58	84	22	77	original
6806	62 [812; D-Xylofuranose (4' 85 [528; Methylcitric acid (4TMS)]	0.452	0.614	9.203	0.502	46	96	58	84	22	77	original
6831	62 [812; D-Xylofuranose (4' 110 [715; Erythritol (4TMS)]	0.451	0.781	17.864	0.645	47	95	34	108	87	14	original
6856	62 [812; D-Xylofuranose (4' 902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	0.448	0.584	3.645	0.507	48	94	61	81	1	76	original
6843	62 [812; D-Xylofuranose (4' 122 [644; Erythritol (4TMS)]	0.448	0.780	22.989	0.606	49	93	36	106	116	33	original
6812	62 [812; D-Xylofuranose (4' 91 [766; beta-D-Methylglucopyranoside (4TMS)]	0.443	0.610	16.743	0.435	50	92	59	83	80	112	original
6826	62 [812; D-Xylofuranose (4' 105 [705; 2-Ketogluconic acid (5TMS)]	0.441	0.690	11.779	0.603	51	91	50	92	36	35	original
6834	62 [812; D-Xylofuranose (4' 113 Galactose-6-phosphate	0.436	0.780	15.489	0.562	52	90	33	109	89	55	original
12231	62 [812; D-Xylofuranose (4' 18 [590; 1-Acetyl-2-thiohydantoin]	0.433	0.596	8.466	0.447	53	89	60	82	21	106	duplicate
6818	62 [812; D-Xylofuranose (4' 97 [756; beta-D-Methylglucopyranoside (4TMS)]	0.430	0.739	13.622	0.559	54	88	43	99	55	56	original
10004	62 [812; D-Xylofuranose (4' 1 [938; Sulfuric acid (2TMS)]	0.419	0.580	13.364	0.559	55	87	63	79	52	39	duplicate
6808	62 [812; D-Xylofuranose (4' 87 [945; beta-D-Glucopyranose (5TMS)]	0.414	0.746	22.945	0.500	56	86	40	102	115	78	original
6849	62 [812; D-Xylofuranose (4' 128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	0.404	0.751	9.485	0.634	57	85	39	103	24	16	original
12353	62 [812; D-Xylofuranose (4' 19 Alanine (BP) (3TMS)	0.393	0.681	5.884	0.518	58	84	49	83	11	72	duplicate
10689	62 [812; D-Xylofuranose (4' 6 Glycerol	0.389	0.735	28.936	0.510	59	83	45	87	138	74	duplicate
6837	62 [812; D-Xylofuranose (4' 116 [882; Pseudouridine (5TMS)]	0.389	0.241	12.775	0.445	60	82	76	66	49	107	original
6795	62 [812; D-Xylofuranose (4' 74 [912; Tetradecanoic acid (1TMS)]	0.384	0.584	15.383	0.450	61	81	62	80	68	103	original
15078	62 [812; D-Xylofuranose (4' 44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	0.383	0.692	11.838	0.629	62	80	48	94	37	18	duplicate
6835	62 [812; D-Xylofuranose (4' 114 Fructose-6-phosphate	0.382	0.775	15.762	0.571	63	79	38	104	72	53	original
6847	62 [812; D-Xylofuranose (4' 126 [559; Erythritol (4TMS)]	0.343	0.535	15.004	0.670	64	78	65	77	63	2	original
14784	62 [812; D-Xylofuranose (4' 41 [639; Proline (2TMS)]	0.320	0.528	4.548	0.496	65	77	66	76	4	81	duplicate
6844	62 [812; D-Xylofuranose (4' 123 [945; Galactofuranose-6-phosphate (7TMS)]	0.308	0.575	5.342	0.537	66	76	84	78	7	67	original
6825	62 [812; D-Xylofuranose (4' 104 [795; Erythritol (4TMS)]	0.306	0.512	11.993	0.495	67	75	68	74	40	83	original
6817	62 [812; D-Xylofuranose (4' 96 myo-Inositol	0.287	0.244	26.882	0.297	68	74	75	67	128	140	original
6801	62 [812; D-Xylofuranose (4' 80 [772; D-Glucose (5TMS)]	0.263	0.648	18.659	0.468	69	73	54	88	89	94	original
6804	62 [812; D-Xylofuranose (4' 83 Sorbitol	0.260	-0.237	12.024	0.331	70	72	92	50	41	138	original
6848	62 [812; D-Xylofuranose (4' 127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	0.250	0.522	11.250	0.665	71	71	67	75	33	6	original
6785	62 [812; D-Xylofuranose (4' 64 [789; Tyramine (3TMS)]	0.210	0.408	12.739	0.448	72	70	70	72	47	105	original
6805	62 [812; D-Xylofuranose (4' 84 Mannitol	0.186	0.401	20.110	0.428	73	69	71	71	99	117	original
11859	62 [812; D-Xylofuranose (4' 15 Alanine	0.184	0.449	7.520	0.605	74	68	89	73	17	34	duplicate
6812	62 [812; D-Xylofuranose (4' 140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	0.151	0.118	23.219	0.625	75	67	81	61	117	118	original
15383	62 [812; D-Xylofuranose (4' 47 [NA]	0.147	0.157	14.539	0.412	76	65	79	63	60	122	duplicate
6854	62 [812; D-Xylofuranose (4' 133 [855; Squalene]	0.147	0.055	12.086	0.389	77	66	83	59	42	130	original
6832	62 [812; D-Xylofuranose (4' 111 [583; Erythritol (4TMS)]	0.136	0.297	27.993	0.484	78	64	74	68	133	85	original
6800	62 [812; D-Xylofuranose (4' 79 Glucose	0.129	0.639	22.172	0.544	79	63	56	86	109	62	original

6830	62 [812; D-Xylofuranose (4' 108	Octadecanoic acid	64	0.109	0.330	13.477	0.472	80	62	73	69	53	91 original
6815	62 [812; D-Xylofuranose (4' 94	Hexadecanoic acid	64	0.037	0.234	10.926	0.460	81	61	77	65	31	98 original
6814	62 [812; D-Xylofuranose (4' 93	Putrescine (4TMS)]	60	0.035	0.148	25.012	0.381	82	60	80	82	122	133 original
6862	62 [812; D-Xylofuranose (4' 141	Lanosta-9,24-dien-3-beta-ol	61	0.030	-0.004	22.387	0.434	83	59	84	58	111	113 original
6860	62 [812; D-Xylofuranose (4' 139	Ergosta-5,7-dien-3-ol	38	0.027	-0.112	24.879	0.420	84	58	86	58	121	119 original
6839	62 [812; D-Xylofuranose (4' 118	[928; Glucopyranose-6-phosphate (6TMS)]	58	0.022	0.186	16.045	0.463	85	57	78	64	75	97 original
6859	62 [812; D-Xylofuranose (4' 138	Ergosterol (1TMS)]	46	-0.007	0.058	23.705	0.409	86	58	82	60	118	124 original
15906	62 [812; D-Xylofuranose (4' 53	Glycerol-2-phosphate	64	-0.026	-0.066	19.820	0.360	87	55	85	57	96	136 duplicate
6811	62 [812; D-Xylofuranose (4' 90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	64	-0.038	-0.156	10.752	0.410	88	54	87	55	28	123 original
6793	62 [812; D-Xylofuranose (4' 72	[919; D-Xylopyranose (4TMS)]	63	-0.056	-0.173	16.662	0.327	89	53	89	53	78	139 original
6858	62 [812; D-Xylofuranose (4' 137	Ergosterol	64	-0.064	-0.203	10.891	0.432	90	52	90	52	29	115 original
6792	62 [812; D-Xylofuranose (4' 71	[731; Erythrose (3TMS)]	64	-0.066	-0.160	5.110	0.415	91	51	88	54	6	121 original
6840	62 [812; D-Xylofuranose (4' 119	[931; myc-Inositol-2-phosphate (7TMS)]	64	-0.078	-0.215	11.893	0.454	92	50	91	51	38	101 original
6828	62 [812; D-Xylofuranose (4' 107	9-(Z)-Octadecenoic acid	64	-0.117	-0.330	6.021	0.419	93	48	95	47	13	120 original
10418	62 [812; D-Xylofuranose (4' 4	Phosphoric acid	51	-0.159	-0.343	22.855	0.291	94	48	96	46	113	141 duplicate
6845	62 [812; D-Xylofuranose (4' 124	[734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	58	-0.198	-0.384	32.572	0.390	95	47	98	44	140	129 original
6851	62 [812; D-Xylofuranose (4' 130	Trehalose	63	-0.216	-0.268	17.603	0.394	96	46	93	49	85	127 original
14981	62 [812; D-Xylofuranose (4' 43	[548; Leucine (2TBS)]	60	-0.228	-0.378	10.906	0.463	97	45	97	45	30	98 duplicate
6804	62 [812; D-Xylofuranose (4' 58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	-0.243	-0.290	9.300	0.385	98	44	94	48	23	132 duplicate
6857	62 [812; D-Xylofuranose (4' 136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.250	-0.483	7.451	0.550	99	43	102	40	15	60 original
6784	62 [812; D-Xylofuranose (4' 63	Glutamine	52	-0.265	-0.752	22.516	0.826	100	42	128	14	112	19 original
14274	62 [812; D-Xylofuranose (4' 36	[596; N-Acetylglutamic acid (2TMS)]	64	-0.277	-0.489	17.516	0.440	101	41	103	39	84	110 duplicate
6796	62 [812; D-Xylofuranose (4' 75	Lysine	64	-0.280	-0.431	27.649	0.381	102	40	89	43	132	135 original
6829	62 [812; D-Xylofuranose (4' 108	Octadecenoic acid	64	-0.285	-0.496	15.820	0.389	103	39	104	38	73	131 original
16647	62 [812; D-Xylofuranose (4' 61	[NA]	64	-0.308	-0.441	12.321	0.463	104	38	100	42	46	86 duplicate
15818	62 [812; D-Xylofuranose (4' 52	[NA]	46	-0.306	-0.683	26.988	0.577	105	37	119	23	129	50 duplicate
10823	62 [812; D-Xylofuranose (4' 7	Threonine	64	-0.311	-0.461	18.045	0.381	106	36	101	41	88	134 duplicate
6819	62 [812; D-Xylofuranose (4' 98	[697; Ribose-5-phosphate methoxamine (5TMS)]	48	-0.321	-0.691	26.777	0.508	107	35	121	21	127	75 original
13293	62 [812; D-Xylofuranose (4' 27	[915; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	-0.347	-0.728	26.036	0.555	108	34	124	18	125	58 duplicate
6787	62 [812; D-Xylofuranose (4' 68	Glyceric acid-3-phosphate	64	-0.363	-0.536	15.056	0.450	109	33	105	37	64	104 original
6788	62 [812; D-Xylofuranose (4' 67	Citric acid	64	-0.377	-0.545	11.723	0.431	110	32	107	35	35	116 original
10143	62 [812; D-Xylofuranose (4' 2	Serine	62	-0.402	-0.570	16.144	0.399	111	31	109	33	76	126 duplicate
12831	62 [812; D-Xylofuranose (4' 23	Homoserine	64	-0.416	-0.757	15.154	0.578	112	30	129	13	66	48 duplicate
18567	62 [812; D-Xylofuranose (4' 60	Glycerol-3-phosphate	64	-0.431	-0.593	10.552	0.468	113	29	112	30	26	93 duplicate
14378	62 [812; D-Xylofuranose (4' 37	Phenylalanine	64	-0.436	-0.626	11.139	0.444	114	28	115	27	32	108 duplicate
15548	62 [812; D-Xylofuranose (4' 49	[877; Pyrophosphoric acid (4TMS)]	64	-0.438	-0.587	29.394	0.459	115	27	111	31	138	99 duplicate
13064	62 [812; D-Xylofuranose (4' 25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.440	-0.834	22.359	0.620	116	26	133	9	110	23 duplicate
15174	62 [812; D-Xylofuranose (4' 45	Homocysteine	61	-0.450	-0.575	30.797	0.437	117	25	110	32	139	111 duplicate
14063	62 [812; D-Xylofuranose (4' 34	Aspartic acid	64	-0.477	-0.541	21.574	0.457	118	24	106	36	104	100 duplicate
11088	62 [812; D-Xylofuranose (4' 9	Proline	63	-0.508	-0.605	20.897	0.404	119	23	113	29	102	125 duplicate
6810	62 [812; D-Xylofuranose (4' 89	[775; Dopamine (4TMS)]	35	-0.509	-0.862	21.699	0.534	120	22	137	5	106	70 original
6852	62 [812; D-Xylofuranose (4' 131	[626; 5-Methylthioadenosine (3TMS)]	55	-0.511	-0.677	25.052	0.534	121	21	118	24	123	69 original
13739	62 [812; D-Xylofuranose (4' 31	[622; Parabanic acid (2TMS)]	64	-0.516	-0.686	19.949	0.540	122	20	120	22	98	64 duplicate
10956	62 [812; D-Xylofuranose (4' 8	Isoleucine	55	-0.522	-0.561	14.923	0.347	123	19	108	34	61	137 duplicate
6816	62 [812; D-Xylofuranose (4' 95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	-0.531	-0.711	27.305	0.442	124	18	122	20	130	109 original
6789	62 [812; D-Xylofuranose (4' 68	[570; Hypoxanthine (2TMS)]	20	-0.537	-0.884	18.743	0.474	125	17	139	3	90	89 original
13048	62 [812; D-Xylofuranose (4' 32	[729; N,N-Dimethyllysine methyl ester]	63	-0.544	-0.743	24.157	0.584	126	16	126	16	120	46 duplicate
13956	62 [812; D-Xylofuranose (4' 33	Methionine	64	-0.550	-0.640	15.143	0.465	127	14	117	25	65	95 duplicate
15456	62 [812; D-Xylofuranose (4' 48	Asparagine	64	-0.550	-0.831	16.758	0.612	128	15	132	10	81	26 duplicate

10281	62 [812; D-Xylofuranose (4'	3	Ethanolamine	62 -0.560	-0.803	20,233	0.540	129	13	131	11	101	63 duplicate
13829	62 [812; D-Xylofuranose (4'	30	[815; Ethyl-3(2H)-thiophenone]	64 -0.583	-0.610	20,149	0.391	130	12	114	28	100	128 duplicate
15729	62 [812; D-Xylofuranose (4'	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44 -0.586	-0.745	26,581	0.487	131	11	127	15	126	84 duplicate
16486	62 [812; D-Xylofuranose (4'	59	Ornithine; Arginine	64 -0.605	-0.630	29,073	0.450	132	10	116	26	137	102 duplicate
6798	62 [812; D-Xylofuranose (4'	77	[826; beta-[(5-methyl-2-thienyl)methyleneamino-benzeneacetic acid methyl ester]	62 -0.612	-0.738	21,473	0.432	133	9	125	17	103	114 original
6790	62 [812; D-Xylofuranose (4'	69	Arginine	60 -0.614	-0.836	15,557	0.593	134	8	134	8	70	42 original
6802	62 [812; D-Xylofuranose (4'	81	Tyrosine	64 -0.614	-0.839	24,033	0.576	135	7	135	7	119	51 original
16079	62 [812; D-Xylofuranose (4'	55	[812; 4-Aminobutyric acid (2TBS)]	43 -0.617	-0.850	28,542	0.496	136	6	136	6	135	80 duplicate
6803	62 [812; D-Xylofuranose (4'	82	Lysine	39 -0.622	-0.905	14,943	0.612	137	5	141	1	62	27 original
12474	62 [812; D-Xylofuranose (4'	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31 -0.639	-0.880	19,862	0.577	138	4	138	4	97	49 duplicate
10554	62 [812; D-Xylofuranose (4'	5	Leucine	45 -0.648	-0.714	15,938	0.500	139	3	123	19	74	79 duplicate
11219	62 [812; D-Xylofuranose (4'	10	Glycine	64 -0.657	-0.900	12,171	0.646	140	2	140	2	44	12 duplicate
14883	62 [812; D-Xylofuranose (4'	42	Glutamic acid	60 -0.692	-0.758	22,859	0.476	141	1	130	12	114	88 duplicate
15819	63 Glutamine	52	[NA]	41 0.763	0.960	10,651	0.645	1	141	2	140	5	19 duplicate
6888	63 Glutamine	89	[775; Dopamine (4TMS)]	31 0.759	0.984	8,343	0.566	2	140	1	141	1	52 original
6887	63 Glutamine	68	[570; Hypoxanthine (2TMS)]	20 0.695	0.954	16,684	0.553	3	139	3	139	46	60 original
6894	63 Glutamine	95	[770; 3,4,6-Trisubstitutedphenylthandamine (5TMS)]	38 0.587	0.717	15,644	0.512	4	138	12	130	37	73 original
16080	63 Glutamine	55	[812; 4-Aminobutyric acid (2TBS)]	32 0.558	0.806	14,734	0.561	5	137	4	138	29	55 duplicate
6904	63 Glutamine	105	[705; 2-Ketogluconic acid (5TMS)]	36 0.556	0.821	19,382	0.579	6	136	7	135	70	45 original
16648	63 Glutamine	61	[NA]	52 0.534	0.731	13,135	0.505	7	135	10	132	18	78 duplicate
6930	63 Glutamine	131	[626; 5-Methylthiadenosine (3TMS)]	43 0.515	0.718	12,950	0.513	8	134	11	131	15	72 original
15457	63 Glutamine	48	Asparagine	52 0.460	0.804	10,113	0.654	9	133	8	134	3	15 duplicate
6881	63 Glutamine	82	Lysine	32 0.460	0.871	10,882	0.642	10	132	6	136	6	20 original
10005	63 Glutamine	1	[838; Sulfuric acid (2TMS)]	35 0.455	0.057	12,254	0.548	11	131	59	83	11	61 duplicate
15549	63 Glutamine	49	[877; Pyrophosphoric acid (4TMS)]	52 0.454	0.603	14,732	0.413	12	130	15	127	28	107 duplicate
6897	63 Glutamine	98	[697; Ribose-5-phosphate methoxamine (5TMS)]	37 0.423	0.580	16,506	0.486	13	129	17	125	44	80 original
15730	63 Glutamine	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	33 0.405	0.573	17,741	0.476	14	128	19	123	55	84 duplicate
10555	63 Glutamine	5	Leucine	34 0.405	0.530	11,806	0.412	15	127	23	119	8	108 duplicate
15175	63 Glutamine	45	Homocysteine	49 0.357	0.456	18,401	0.387	16	126	28	114	58	116 duplicate
6889	63 Glutamine	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	52 0.353	0.478	14,706	0.418	17	125	26	116	27	104 original
6892	63 Glutamine	93	[607; Putrescine (4TMS)]	48 0.348	0.099	15,276	0.419	18	124	55	87	33	101 original
12832	63 Glutamine	23	Homoserine	52 0.338	0.545	12,679	0.546	19	123	21	121	13	62 duplicate
6906	63 Glutamine	107	9-(Z)-Octadecenoic acid	52 0.329	0.536	20,042	0.346	20	122	22	120	76	132 original
13065	63 Glutamine	25	[709; 2,5-Diaminovalerolactam (2TMS)]	38 0.317	0.184	11,810	0.578	21	121	50	92	9	47 duplicate
16322	63 Glutamine	57	[757; 2-Desoxy-pentos-3-yose dimethoxamine (2TMS)]	43 0.311	-0.666	25,827	0.666	22	120	109	33	104	13 duplicate
15907	63 Glutamine	53	Glycerol-2-phosphate	52 0.305	0.313	13,642	0.361	23	119	39	103	20	126 duplicate
6898	63 Glutamine	99	[662; Ribose-5-phosphate methoxamine (BP) (5TMS)]	39 0.298	-0.344	13,624	0.587	24	118	74	68	19	43 original
6918	63 Glutamine	119	[931; myo-Inositol-2-phosphata (7TMS)]	52 0.282	0.599	14,322	0.463	25	117	16	126	24	88 original
6868	63 Glutamine	69	Arginine	48 0.282	0.588	20,342	0.628	26	116	18	124	80	26 original
13957	63 Glutamine	33	Methionine	52 0.267	0.415	14,074	0.426	27	115	34	108	22	98 duplicate
14982	63 Glutamine	43	[548; Leucine (2TBS)]	48 0.262	0.196	14,754	0.488	28	114	47	85	30	79 duplicate
14064	63 Glutamine	34	Aspartic acid	52 0.261	0.387	33,353	0.414	29	113	38	104	126	105 duplicate
13630	63 Glutamine	30	[815; Ethyl-3(2H)-thiophenone]	52 0.256	0.403	29,815	0.366	30	112	37	105	117	124 duplicate
10282	63 Glutamine	3	Ethanolamine	50 0.241	0.712	10,488	0.606	31	111	13	129	4	41 duplicate
12475	63 Glutamine	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	24 0.239	0.876	11,739	0.641	32	110	5	137	7	21 duplicate
6927	63 Glutamine	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	38 0.232	-0.014	17,120	0.621	33	109	62	80	51	34 original
6893	63 Glutamine	84	Mannitol	50 0.231	-0.020	35,821	0.437	34	108	63	79	132	95 original

6907	63	Glutamine	108	Octadecanoic acid	52	0.231	0.411	13,006	0.377	35	107	35	107	16	120 original
6896	63	Glutamine	97	[756; beta-D-Methylglucopyranoside (4TMS)]	40	0.228	-0.371	30,463	0.579	36	108	76	68	119	44 original
6868	63	Glutamine	67	Citric acid	52	0.228	0.522	27,432	0.445	37	105	24	118	113	94 original
11220	63	Glutamine	10	Glycine	52	0.226	0.737	20,018	0.878	38	104	9	133	75	10 duplicate
6876	63	Glutamine	77	[826; beta-[[[5-methyl-2-thienyl]methyleneamino-benzeneacetic acid methyl ester]	50	0.211	0.521	28,841	0.467	39	103	25	117	118	88 original
13294	63	Glutamine	27	[815; (E)-4-Methyl-5-hydroxy-3-pentan-2-one (1TMS)]	41	0.207	0.453	16,738	0.457	40	102	29	113	48	92 duplicate
13740	63	Glutamine	31	[622; Parabenic acid (2TMS)]	52	0.199	0.411	13,094	0.479	41	101	36	106	17	81 duplicate
10957	63	Glutamine	8	Isoleucine	43	0.192	0.231	20,445	0.261	42	100	43	99	82	140 duplicate
14379	63	Glutamine	37	Phenylalanine	52	0.173	0.442	26,285	0.460	43	99	31	111	108	89 duplicate
6880	63	Glutamine	81	Tyrosine	52	0.169	0.657	33,385	0.625	44	98	14	128	127	31 original
15994	63	Glutamine	54	[NA]	43	0.161	-0.522	17,154	0.617	45	97	89	53	53	37 duplicate
14884	63	Glutamine	42	Glutamic acid	48	0.156	0.457	27,138	0.428	46	96	27	115	111	97 duplicate
16487	63	Glutamine	59	Ornithine; Arginine	52	0.143	0.421	40,858	0.457	47	95	33	109	139	93 duplicate
6926	63	Glutamine	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	34	0.137	0.559	12,124	0.653	48	94	20	122	10	16 original
6871	63	Glutamine	72	[918; D-Xylopyranose (4TMS)]	51	0.112	0.116	14,790	0.318	49	93	51	91	31	136 original
11089	63	Glutamine	9	Proline	51	0.106	0.282	27,253	0.353	50	92	41	101	112	130 duplicate
6865	63	Glutamine	66	Glycine acid-3-phosphate	52	0.085	0.265	13,643	0.398	51	91	42	100	21	111 original
13849	63	Glutamine	32	[728; N,N-Dimethyllysine methyl ester]	51	0.089	0.447	14,427	0.542	52	90	30	112	26	64 duplicate
16568	63	Glutamine	60	Glycerol-3-phosphate	52	0.084	0.421	25,290	0.466	53	89	32	110	100	87 duplicate
15364	63	Glutamine	47	[NA]	52	0.071	-0.084	18,059	0.458	54	88	65	77	57	91 duplicate
6891	63	Glutamine	128	[680; Glycerol-2-phosphate (4TMS)]	42	0.064	-0.757	18,313	0.628	55	87	123	19	68	27 original
6928	63	Glutamine	124	[734; 1-Monooctadecyglycerol (2TMS); 1-Monohexadecyglycerol (1TMS)]	47	0.047	-0.683	23,599	0.673	56	86	114	28	94	11 original
6923	63	Glutamine	65	[646; 3-Deoxyglucitol (5TMS)]	49	0.020	0.295	20,111	0.391	57	85	40	102	77	114 original
10144	63	Glutamine	2	Serine	51	0.020	-0.756	28,078	0.724	58	84	122	20	105	1 original
6938	63	Glutamine	137	Ergosterol	50	0.001	0.207	20,795	0.355	59	83	45	97	84	129 duplicate
10824	63	Glutamine	7	Threonine	52	-0.011	0.205	20,157	0.385	60	82	46	98	78	118 original
12949	63	Glutamine	24	[725; 2-Ketooctanoic acid (2TMS)]	52	-0.015	0.211	32,535	0.369	61	81	44	98	123	123 duplicate
11985	63	Glutamine	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	52	-0.026	-0.700	37,890	0.717	62	80	116	26	134	3 duplicate
15840	63	Glutamine	50	[746; Ribonic acid-1,4-lactone (3TMS)]	52	-0.030	-0.663	26,383	0.698	63	79	107	35	107	6 duplicate
15270	63	Glutamine	46	Arabinose	49	-0.032	-0.610	18,880	0.825	64	78	96	48	61	30 duplicate
13519	63	Glutamine	29	Erythritol	52	-0.039	-0.770	30,452	0.723	65	77	126	16	118	2 duplicate
12109	63	Glutamine	17	[700; 2-methyl-1,2-propanediol (2TMS)]	52	-0.053	-0.610	16,468	0.622	66	75	97	45	41	32 duplicate
6870	63	Glutamine	71	[731; Erythrose (3TMS)]	52	-0.063	-0.659	26,646	0.621	67	76	105	37	109	33 duplicate
14275	63	Glutamine	36	[596; N-Acetylglutamic acid (2TMS)]	52	-0.062	0.108	18,956	0.359	68	74	53	89	63	127 original
16238	63	Glutamine	56	[929; Orolic acid (3TMS)]	52	-0.072	-0.187	30,680	0.344	69	73	49	93	121	134 duplicate
6938	63	Glutamine	139	[700; Ergosta-5,7-dien-3-ol]	52	-0.074	-0.763	23,621	0.705	70	72	124	18	95	5 duplicate
6929	63	Glutamine	130	Trehalose	36	-0.079	0.094	16,547	0.396	71	71	57	85	45	113 original
6940	63	Glutamine	141	Lanosta-8,24-dien-3-beta-ol	51	-0.082	0.101	32,550	0.365	72	70	54	88	124	125 original
11607	63	Glutamine	13	Uracil	49	-0.088	0.188	14,391	0.431	73	69	48	94	25	98 original
14584	63	Glutamine	88	Gluconic acid	52	-0.092	-0.688	26,587	0.698	74	68	115	27	108	7 duplicate
6933	63	Glutamine	39	[829; 1-Phenylmethanol (1TMS)]	52	-0.095	-0.681	24,055	0.647	75	67	113	29	97	18 original
11479	63	Glutamine	134	Isomaltose	51	-0.100	-0.721	28,274	0.687	76	66	119	23	114	8 duplicate
6885	63	Glutamine	12	Glyceric acid	52	-0.106	-0.755	35,281	0.698	77	65	121	21	130	8 original
6919	63	Glutamine	86	[793; D-Galactono-1,4-lactone (4TMS)]	51	-0.115	-0.521	18,079	0.545	78	64	88	54	39	63 duplicate
6902	63	Glutamine	120	[945; Uridine (3TMS)]	49	-0.122	-0.814	34,647	0.707	79	63	131	11	129	4 original
6890	63	Glutamine	103	[648; Ethylamine (2TMS)]	43	-0.132	-0.143	19,428	0.632	80	62	67	75	71	25 original
			91	[766; beta-D-Methylglucopyranoside (4TMS)]	51	-0.151	-0.551	25,807	0.558	81	61	92	50	103	57 original
					52	-0.152	-0.411	27,015	0.506	82	60	78	64	110	75 original

14482	63	Glutamine	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	52	-0.154	-0.665	19.074	0.627	83	59	108	34	64	28	Juplicate
10419	63	Glutamine	4	Phosphoric acid	39	-0.163	0.059	32.986	0.200	84	58	58	84	125	141	Juplicate
6900	63	Glutamine	101	[832; Dopamine (4TMS)]	52	-0.167	-0.469	21.929	0.540	85	57	82	60	87	65	original
11350	63	Glutamine	11	Succinic acid	52	-0.176	-0.652	18.436	0.621	86	56	104	38	59	35	Juplicate
6874	63	Glutamine	75	Lysine	52	-0.195	0.095	40.122	0.349	87	55	56	86	138	131	original
12714	63	Glutamine	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	41	-0.205	-0.534	16.169	0.561	88	54	90	52	40	54	Juplicate
6893	63	Glutamine	94	Hexadecanoic acid	52	-0.207	-0.230	28.297	0.397	89	53	70	72	115	112	original
15079	63	Glutamine	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	38	-0.215	-0.376	19.437	0.587	90	52	77	65	72	42	Juplicate
6939	63	Glutamine	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	43	-0.236	-0.078	16.495	0.389	91	51	64	78	43	115	original
6934	63	Glutamine	135	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	52	-0.237	-0.303	19.614	0.419	92	50	71	71	73	102	original
6882	63	Glutamine	83	Sorbitol	46	-0.241	0.010	24.502	0.298	93	49	60	82	99	139	original
6921	63	Glutamine	122	[644; Erythritol (4TMS)]	40	-0.244	-0.428	15.319	0.573	94	48	79	63	34	51	original
6908	63	Glutamine	109	Oxaladecanoic acid	52	-0.252	-0.352	30.465	0.425	96	46	75	67	120	99	original
6925	63	Glutamine	126	[559; Erythritol (4TMS)]	35	-0.264	0.113	12.521	0.577	97	45	52	90	12	49	original
16727	63	Glutamine	62	[812; D-Xylofuranose (4TMS)]	52	-0.265	-0.752	22.516	0.626	98	44	120	22	90	29	Juplicate
6910	63	Glutamine	111	[583; Erythritol (4TMS)]	36	-0.267	-0.321	14.077	0.356	99	43	72	70	23	128	original
6911	63	Glutamine	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	52	-0.267	-0.438	16.999	0.471	100	42	80	62	50	85	original
16405	63	Glutamine	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	52	-0.273	0.002	21.060	0.318	101	41	61	81	85	137	Juplicate
12595	63	Glutamine	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	-0.282	-0.541	24.086	0.460	102	40	91	51	98	90	Juplicate
6931	63	Glutamine	132	[695; Isomaltose methoxyamine (8TMS)]	36	-0.289	-0.561	15.815	0.614	103	39	93	49	38	38	original
6895	63	Glutamine	96	myo-Inositol	41	-0.305	-0.323	19.250	0.345	104	38	73	69	67	133	original
6932	63	Glutamine	133	[655; Squalene]	52	-0.317	-0.185	17.148	0.334	105	37	68	74	52	135	original
6937	63	Glutamine	138	[674; Ergosterol (1TMS)]	43	-0.318	-0.205	16.972	0.375	106	38	69	73	49	121	original
6872	63	Glutamine	73	[708; Glucose methoxyamine (5TMS)]	45	-0.321	-0.704	21.845	0.522	107	35	117	25	86	70	original
6886	63	Glutamine	87	[945; beta-D-Glucopyranose (5TMS)]	50	-0.322	-0.811	40.102	0.532	108	34	129	13	137	68	original
11734	63	Glutamine	14	Fumaric acid	52	-0.332	-0.670	16.492	0.613	109	33	110	32	42	39	Juplicate
6924	63	Glutamine	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	52	-0.333	-0.894	37.922	0.640	110	32	139	3	135	23	original
6901	63	Glutamine	102	[904; Galactose methoxyamine (5TMS)]	52	-0.354	-0.444	15.642	0.513	111	31	81	61	36	71	original
13180	63	Glutamine	26	Citramalic acid	52	-0.356	-0.626	22.965	0.478	112	30	99	43	93	83	Juplicate
6909	63	Glutamine	110	[715; Erythritol (4TMS)]	42	-0.357	-0.663	19.960	0.633	113	29	106	38	74	24	original
12232	63	Glutamine	18	[590; 1-Acetyl-2-thiohydantoin]	52	-0.359	-0.493	17.961	0.370	114	28	84	58	56	122	Juplicate
6884	63	Glutamine	85	[529; Methylidic acid (4TMS)]	36	-0.365	-0.489	14.857	0.313	115	27	83	59	32	138	original
6917	63	Glutamine	118	[928; Glucopyranose-6-phosphate (6TMS)]	47	-0.365	-0.564	17.608	0.418	116	26	94	48	54	103	original
14885	63	Glutamine	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	52	-0.382	-0.632	37.445	0.575	117	25	100	42	133	50	Juplicate
13407	63	Glutamine	28	Malic acid	52	-0.386	-0.671	19.162	0.620	118	24	111	31	66	36	Juplicate
6899	63	Glutamine	100	[657; Mannitol (6TMS)]	52	-0.403	-0.497	18.525	0.528	119	23	85	57	60	69	original
10690	63	Glutamine	6	Glycerol	52	-0.418	-0.840	43.740	0.538	120	22	133	9	140	66	Juplicate
6879	63	Glutamine	80	[772; D-Glucose (5TMS)]	50	-0.422	-0.798	35.770	0.488	121	21	127	15	131	78	original
6869	63	Glutamine	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	46	-0.422	-0.707	25.575	0.491	122	20	118	24	102	77	original
6915	63	Glutamine	116	[882; Pseudouridine (5TMS)]	27	-0.430	-0.138	12.814	0.378	123	19	68	76	14	119	original
6916	63	Glutamine	117	[724; Glycerol (3TMS)]	46	-0.443	-0.620	19.157	0.556	124	18	98	44	65	58	original
6877	63	Glutamine	78	Mannose	51	-0.448	-0.798	22.715	0.561	125	17	128	14	92	56	original
6935	63	Glutamine	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.456	-0.805	9.348	0.410	126	16	95	47	2	109	original
6920	63	Glutamine	121	[657; Erythritol (4TMS)]	44	-0.467	-0.650	16.707	0.578	127	15	103	39	47	48	original
6873	63	Glutamine	74	[912; Tetradecanoic acid (1TMS)]	52	-0.471	-0.515	20.489	0.413	128	14	88	58	83	106	original
6875	63	Glutamine	76	Fructose	52	-0.472	-0.868	34.295	0.640	129	13	136	6	128	22	original
6863	63	Glutamine	64	[789; Tyramine (3TMS)]	51	-0.475	-0.650	15.516	0.408	130	12	102	40	35	110	original
6905	63	Glutamine	106	[733; Threitol (4TMS)]	52	-0.483	-0.767	23.924	0.658	131	11	125	17	98	14	original
14170	63	Glutamine	35	Pyroglutamic acid	52	-0.496	-0.877	44.056	0.688	132	10	137	5	141	12	Juplicate

6903	63	Glutamine	104	[795; Erythritol (4TMS)]	51	-0.506	-0.641	19.315	0.506	133	9	101	41	69	74 original
6914	63	Glutamine	115	Glucose-6-phosphate	51	-0.515	-0.863	32.014	0.647	134	8	134	8	122	17 original
14765	63	Glutamine	41	[639; Proline (2TMS)]	52	-0.573	-0.872	22.480	0.422	135	7	112	30	89	100 duplicate
6912	63	Glutamine	113	Galactose-6-phosphate	51	-0.580	-0.879	20.387	0.553	136	6	138	4	81	59 original
11860	63	Glutamine	15	Alanine	52	-0.609	-0.925	25.366	0.607	137	5	141	1	101	40 duplicate
6913	63	Glutamine	114	Fructose-6-phosphate	48	-0.640	-0.864	18.906	0.578	138	4	135	7	62	46 original
12354	63	Glutamine	19	Alanine (BP) (3TMS)	52	-0.643	-0.813	22.597	0.478	139	3	130	12	91	82 duplicate
6878	63	Glutamine	79	Glucose	52	-0.656	-0.923	38.433	0.564	140	2	140	2	136	53 original
6922	63	Glutamine	123	[945; Galactofuranose-6-phosphate (7TMS)]	52	-0.679	-0.822	20.195	0.534	141	1	132	10	79	67 original
11861	64	[789; Tyramine (3TMS)]	15	Alanine	63	0.656	0.802	17.023	0.480	1	141	1	141	93	6 duplicate
6955	64	[789; Tyramine (3TMS)]	79	Glucose	63	0.546	0.725	34.010	0.439	2	140	2	140	138	23 original
6990	64	[789; Tyramine (3TMS)]	114	Fructose-6-phosphate	53	0.512	0.714	6.152	0.449	3	139	3	139	13	16 original
6989	64	[789; Tyramine (3TMS)]	123	[945; Galactofuranose-6-phosphate (7TMS)]	63	0.491	0.683	8.887	0.418	4	138	4	138	33	42 original
6989	64	[789; Tyramine (3TMS)]	113	Galactose-6-phosphate	61	0.496	0.667	6.088	0.452	5	137	5	137	12	12 original
6980	64	[789; Tyramine (3TMS)]	104	[795; Erythritol (4TMS)]	62	0.365	0.445	6.075	0.442	6	136	15	127	11	20 original
12355	64	[789; Tyramine (3TMS)]	19	Alanine (BP) (3TMS)	63	0.337	0.459	10.584	0.397	7	135	13	129	45	68 duplicate
16406	64	[789; Tyramine (3TMS)]	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	63	0.335	0.327	14.808	0.351	8	134	24	118	77	109 duplicate
6951	64	[789; Tyramine (3TMS)]	75	Lysine	63	0.334	0.285	38.771	0.356	9	133	34	108	138	105 original
7001	64	[789; Tyramine (3TMS)]	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	63	0.324	0.601	31.153	0.398	10	132	6	136	129	66 original
14171	64	[789; Tyramine (3TMS)]	35	Pyroglutamic acid	63	0.323	0.557	40.534	0.404	11	131	8	134	140	58 duplicate
6949	64	[789; Tyramine (3TMS)]	73	[708; Glucose methoxamine (5TMS)]	56	0.322	0.453	9.076	0.400	12	130	14	128	34	60 original
6959	64	[789; Tyramine (3TMS)]	83	Sorbitol	57	0.315	0.162	19.950	0.289	13	129	58	84	108	137 original
6991	64	[789; Tyramine (3TMS)]	115	Glucose-6-phosphate	61	0.293	0.569	23.768	0.441	14	128	7	135	118	22 original
14786	64	[789; Tyramine (3TMS)]	41	[639; Proline (2TMS)]	63	0.279	0.294	12.359	0.394	15	127	30	112	60	69 duplicate
6992	64	[789; Tyramine (3TMS)]	116	[882; Pseudouridine (5TMS)]	30	0.269	-0.029	8.279	0.280	16	128	85	47	27	139 original
6972	64	[789; Tyramine (3TMS)]	96	myo-Inositol	48	0.264	0.147	16.151	0.299	17	125	59	83	85	135 original
12233	64	[789; Tyramine (3TMS)]	18	[590; 1-Acetyl-2-thiohydantoin]	63	0.259	0.311	5.878	0.348	18	124	26	116	8	112 duplicate
10691	64	[789; Tyramine (3TMS)]	6	Glycerol	63	0.258	0.505	40.993	0.431	19	123	9	133	141	34 duplicate
13408	64	[789; Tyramine (3TMS)]	28	Malic acid	61	0.248	0.245	7.826	0.416	20	122	38	104	20	45 duplicate
6954	64	[789; Tyramine (3TMS)]	78	Mannose	61	0.246	0.409	9.692	0.380	21	121	17	125	38	81 original
6942	64	[789; Tyramine (3TMS)]	66	Glyceric acid-3-phosphate	63	0.241	0.238	3.867	0.331	22	120	39	103	5	130 original
10825	64	[789; Tyramine (3TMS)]	7	Threonine	63	0.229	0.231	29.237	0.332	23	119	43	99	127	129 duplicate
6987	64	[789; Tyramine (3TMS)]	111	[583; Erythritol (4TMS)]	42	0.222	0.499	17.150	0.392	24	118	10	132	94	71 original
10145	64	[789; Tyramine (3TMS)]	2	Serine	61	0.220	0.092	18.166	0.341	25	117	72	70	103	117 duplicate
6946	64	[789; Tyramine (3TMS)]	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	56	0.217	0.495	17.366	0.386	26	116	11	131	97	75 original
6952	64	[789; Tyramine (3TMS)]	76	Fructose	63	0.211	0.488	24.881	0.421	27	115	12	130	119	39 original
16728	64	[789; Tyramine (3TMS)]	62	[812; D-Xylofuranose (4TMS)]	63	0.210	0.408	12.739	0.448	28	114	18	124	62	18 duplicate
6978	64	[789; Tyramine (3TMS)]	102	[904; Galactose methoxamine (5TMS)]	63	0.204	0.389	3.420	0.409	29	113	19	123	4	53 original
12596	64	[789; Tyramine (3TMS)]	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	63	0.203	0.236	15.452	0.370	30	112	42	100	81	94 duplicate
13181	64	[789; Tyramine (3TMS)]	26	Citramalic acid	63	0.198	0.182	15.074	0.401	31	111	56	88	80	59 duplicate
6982	64	[789; Tyramine (3TMS)]	106	[733; Threitol (4TMS)]	61	0.192	0.341	10.418	0.494	32	110	22	120	43	2 original
7009	64	[789; Tyramine (3TMS)]	133	[855; Squalene]	63	0.184	0.215	6.302	0.365	33	109	48	94	15	97 original
14483	64	[789; Tyramine (3TMS)]	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	63	0.181	0.206	6.414	0.451	34	108	52	90	17	13 duplicate
14686	64	[789; Tyramine (3TMS)]	40	[800; 2,3-Dimethylsuccinic acid (2TMS)]	63	0.178	0.272	33.649	0.353	35	107	36	108	135	106 duplicate
11351	64	[789; Tyramine (3TMS)]	11	Succinic acid	63	0.176	0.338	5.928	0.412	36	106	23	119	10	48 duplicate
7006	64	[789; Tyramine (3TMS)]	130	Trehalose	63	0.175	0.140	29.235	0.366	37	105	60	82	126	96 original
11735	64	[789; Tyramine (3TMS)]	14	Fumaric acid	63	0.167	0.214	6.160	0.371	38	104	50	92	14	91 duplicate
6988	64	[789; Tyramine (3TMS)]	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	62	0.164	0.228	13.395	0.376	39	103	44	98	65	85 original
7011	64	[789; Tyramine (3TMS)]	135	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	63	0.164	0.177	10.659	0.486	40	102	57	85	47	4 original

6962	64 [789; Tyramine (3TMS)]	86 [789; D-Galactono-1,4-lactone (4TMS)]	0.160	0.441	21.776	0.486	41	101	16	126	115	3 original
6976	64 [789; Tyramine (3TMS)]	107 [657; Mannitol (6TMS)]	0.156	0.226	7.181	0.382	42	100	46	96	19	78 original
13295	64 [789; Tyramine (3TMS)]	27 [815; (E)-4-Methyl-5-hydroxy-3-pentan-2-one (1TMS)]	0.152	-0.001	16.955	0.331	43	99	89	53	91	131 duplicate
14276	64 [789; Tyramine (3TMS)]	36 [596; N-Acetylglutamic acid (2TMS)]	0.152	0.112	17.725	0.329	44	98	67	75	122	133 duplicate
16239	64 [789; Tyramine (3TMS)]	56 [829; Oxalic acid (3TMS)]	0.144	0.350	10.625	0.428	45	97	21	121	46	35 duplicate
13520	64 [789; Tyramine (3TMS)]	29 Erythritol	0.141	0.215	3.376	0.435	46	98	49	93	3	29 duplicate
11988	64 [789; Tyramine (3TMS)]	17 [644; 2-Methyl-1,3-butanediol (2TMS)]	0.137	0.221	17.012	0.496	47	95	47	95	92	1 duplicate
12110	64 [789; Tyramine (3TMS)]	17 [700; 2-methyl-1,2-propanediol (2TMS)]	0.131	0.277	16.897	0.384	48	94	35	107	80	76 duplicate
6956	64 [789; Tyramine (3TMS)]	80 [772; D-Glucose (5TMS)]	0.130	0.293	29.959	0.374	49	93	32	110	128	89 original
6961	64 [789; Tyramine (3TMS)]	85 [529; Methylcitric acid (4TMS)]	0.129	0.193	2.796	0.408	50	92	54	88	1	54 original
7014	64 [789; Tyramine (3TMS)]	138 [674; Ergosterol (1TMS)]	0.127	0.237	12.875	0.375	51	91	40	102	63	87 original
10420	64 [789; Tyramine (3TMS)]	4 Phosphoric acid	0.127	0.063	32.156	0.279	52	90	81	61	133	140 duplicate
6947	64 [789; Tyramine (3TMS)]	71 [731; Erythrose (3TMS)]	0.126	0.123	10.568	0.410	53	89	64	78	44	51 original
6974	64 [789; Tyramine (3TMS)]	98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	0.121	0.047	16.531	0.338	54	88	85	57	88	120 original
12950	64 [789; Tyramine (3TMS)]	24 [725; 2-Ketooctanoic acid (2TMS)]	0.120	0.236	31.514	0.449	55	87	41	101	131	17 duplicate
11090	64 [789; Tyramine (3TMS)]	9 Proline	0.117	0.081	26.825	0.319	56	86	76	66	121	134 duplicate
6967	64 [789; Tyramine (3TMS)]	91 [766; beta-D-Methylglucopyranoside (4TMS)]	0.114	0.121	17.370	0.358	57	85	65	77	98	102 original
14565	64 [789; Tyramine (3TMS)]	39 [829; 1-Phenylethanol (1TMS)]	0.111	0.190	16.340	0.389	58	84	55	87	87	73 duplicate
6964	64 [789; Tyramine (3TMS)]	88 Gluconic acid	0.108	0.227	11.688	0.434	59	82	45	97	55	31 original
6977	64 [789; Tyramine (3TMS)]	101 [832; Dopamine (4TMS)]	0.100	0.077	7.903	0.390	60	83	68	74	49	64 original
6994	64 [789; Tyramine (3TMS)]	118 [928; Glucopyranose-6-phosphate (6TMS)]	0.099	0.291	24.917	0.447	62	80	33	109	120	80 original
7010	64 [789; Tyramine (3TMS)]	134 Isomaltose	0.098	0.121	11.820	0.412	63	79	66	76	57	49 original
6997	64 [789; Tyramine (3TMS)]	121 [657; Erythritol (4TMS)]	0.096	0.136	14.470	0.375	64	78	61	81	73	88 original
6979	64 [789; Tyramine (3TMS)]	103 [646; Ethylamine (2TMS)]	0.086	0.033	10.677	0.423	65	77	87	55	48	38 duplicate
12715	64 [789; Tyramine (3TMS)]	22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	0.086	0.352	17.542	0.436	66	76	20	122	99	25 duplicate
15271	64 [789; Tyramine (3TMS)]	46 Arabinose	0.078	0.048	8.111	0.350	67	75	84	58	25	110 duplicate
13741	64 [789; Tyramine (3TMS)]	65 [646; 3-Deoxyglucitol (5TMS)]	0.071	0.317	13.466	0.436	68	74	25	117	68	28 original
14380	64 [789; Tyramine (3TMS)]	37 Phenylalanine	0.070	0.059	21.731	0.375	69	73	79	63	114	88 duplicate
11608	64 [789; Tyramine (3TMS)]	13 Uracil	0.069	0.193	15.765	0.439	70	72	53	89	83	24 duplicate
13850	64 [789; Tyramine (3TMS)]	32 [729; N,N-Dimethyllysine methyl ester]	0.068	0.049	14.534	0.334	72	70	83	59	74	125 duplicate
13066	64 [789; Tyramine (3TMS)]	25 [709; 2,5-Diaminovalerolactam (2TMS)]	0.062	0.293	13.457	0.399	73	69	31	111	67	63 duplicate
12833	64 [789; Tyramine (3TMS)]	23 Homoserine	0.059	-0.009	9.932	0.335	74	68	90	52	41	123 duplicate
6950	64 [789; Tyramine (3TMS)]	74 [912; Tetradecanoic acid (1TMS)]	0.058	0.135	9.703	0.353	75	67	63	79	39	107 original
6963	64 [789; Tyramine (3TMS)]	87 [945; beta-D-Glucopyranose (5TMS)]	0.056	0.303	34.582	0.418	76	66	28	114	137	43 original
6957	64 [789; Tyramine (3TMS)]	81 Tyrosine	0.050	-0.190	33.214	0.486	77	65	115	27	134	5 original
10958	64 [789; Tyramine (3TMS)]	8 Isoleucine	0.043	-0.016	17.980	0.283	78	64	92	50	100	138 duplicate
16488	64 [789; Tyramine (3TMS)]	59 Ornithine; Arginine	0.040	0.086	40.018	0.342	79	62	75	67	139	115 duplicate
13958	64 [789; Tyramine (3TMS)]	33 Methionine	0.040	0.060	9.916	0.339	80	63	82	60	40	118 duplicate
6996	64 [789; Tyramine (3TMS)]	120 [945; Uridine (3TMS)]	0.030	-0.043	10.745	0.399	81	61	99	43	50	62 original
16649	64 [789; Tyramine (3TMS)]	61 [NA]	0.027	-0.034	4.523	0.399	82	60	98	44	6	65 duplicate
11480	64 [789; Tyramine (3TMS)]	12 Glyceralic acid	0.024	0.065	8.284	0.360	83	59	80	62	28	100 duplicate
13631	64 [789; Tyramine (3TMS)]	30 [815; Ethyl-3(2H)-thiophenone]	0.024	0.101	28.962	0.334	84	58	69	73	125	126 duplicate
14983	64 [789; Tyramine (3TMS)]	43 [548; Leucine (2TBS)]	0.018	0.088	6.406	0.352	85	57	74	68	16	108 duplicate
7008	64 [789; Tyramine (3TMS)]	132 [895; Isomaltose methoxyamine (8TMS)]	0.015	-0.020	14.576	0.371	86	56	93	49	75	92 original
14065	64 [789; Tyramine (3TMS)]	34 Aspartic acid	0.012	0.076	31.956	0.331	87	55	78	64	132	132 duplicate
15995	64 [789; Tyramine (3TMS)]	54 [NA]	0.009	0.302	10.777	0.374	88	54	29	113	51	90 duplicate
6943	64 [789; Tyramine (3TMS)]	67 Citric acid	-0.001	-0.057	22.781	0.397	89	52	102	40	117	67 original
16569	64 [789; Tyramine (3TMS)]	60 Glycerol-3-phosphate	-0.001	-0.076	20.459	0.335	90	53	105	37	108	124 duplicate
6993	64 [789; Tyramine (3TMS)]	117 [724; Glycerol (3TMS)]	-0.002	-0.024	8.563	0.383	91	51	94	48	32	77 original

129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]		128 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	
7005	64 [789; Tyramine (3TMS)]	59 -0.004	0.136
10283	64 [789; Tyramine (3TMS)]	61 -0.012	-0.231
7012	64 [789; Tyramine (3TMS)]	17 -0.015	0.092
11221	64 [789; Tyramine (3TMS)]	63 -0.015	-0.188
77 [826; beta-[(5-methyl-2-phenyl)methyl]amino-benzeneacetic acid methyl ester]		61 -0.015	-0.059
6953	64 [789; Tyramine (3TMS)]	61 -0.020	0.089
15941	64 [789; Tyramine (3TMS)]	60 -0.021	-0.014
15176	64 [789; Tyramine (3TMS)]	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	0.047
8975	64 [789; Tyramine (3TMS)]	37 -0.024	-0.236
7015	64 [789; Tyramine (3TMS)]	43 -0.025	-0.051
15731	64 [789; Tyramine (3TMS)]	63 -0.056	0.089
6985	64 [789; Tyramine (3TMS)]	53 -0.060	-0.030
6986	64 [789; Tyramine (3TMS)]	59 -0.060	-0.134
7016	64 [789; Tyramine (3TMS)]	48 -0.073	-0.098
14885	64 [789; Tyramine (3TMS)]	59 -0.074	-0.071
15458	64 [789; Tyramine (3TMS)]	63 -0.079	-0.299
6968	64 [789; Tyramine (3TMS)]	54 -0.086	-0.310
6998	64 [789; Tyramine (3TMS)]	52 -0.094	-0.180
110 [715; Erythritol (4TMS)]		55 -0.108	0.206
6945	64 [789; Tyramine (3TMS)]	62 -0.114	-0.317
7016	64 [789; Tyramine (3TMS)]	63 -0.119	0.023
14885	64 [789; Tyramine (3TMS)]	44 -0.142	-0.053
15458	64 [789; Tyramine (3TMS)]	54 -0.147	-0.302
6968	64 [789; Tyramine (3TMS)]	63 -0.150	-0.253
6998	64 [789; Tyramine (3TMS)]	57 [757; 2-Desoxy-pentose-3-ylose dimethoxyamine (2TMS)]	0.206
16323	64 [789; Tyramine (3TMS)]	72 [919; D-Xylopyranose (4TMS)]	0.436
6948	64 [789; Tyramine (3TMS)]	84 Hexadecanoic acid	0.345
6970	64 [789; Tyramine (3TMS)]	5 Leucine	0.273
10556	64 [789; Tyramine (3TMS)]	131 [626; 5-Methylthioadenosine (3TMS)]	0.273
7007	64 [789; Tyramine (3TMS)]	47 [NA]	0.425
15365	64 [789; Tyramine (3TMS)]	124 [734; 1-Monooleoylglycerol (2TMS); 1-Monoheptadecenoylethanol (1TMS)]	0.334
7000	64 [789; Tyramine (3TMS)]	44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	0.357
15080	64 [789; Tyramine (3TMS)]	108 Octadecanoic acid	0.469
6984	64 [789; Tyramine (3TMS)]	126 [559; Erythritol (4TMS)]	0.367
7002	64 [789; Tyramine (3TMS)]	68 [570; Hypoxanthine (2TMS)]	0.466
6944	64 [789; Tyramine (3TMS)]	97 [756; beta-D-Methylglucopyranoside (4TMS)]	0.290
6973	64 [789; Tyramine (3TMS)]	137 Ergosterol	0.442
7013	64 [789; Tyramine (3TMS)]	84 Mannitol	0.359
6960	64 [789; Tyramine (3TMS)]	55 [612; 4-Aminobutyric acid (2TBS)]	0.359
16081	64 [789; Tyramine (3TMS)]	49 [877; Pyrophosphoric acid (4TMS)]	0.419
15550	64 [789; Tyramine (3TMS)]	127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	0.350
7003	64 [789; Tyramine (3TMS)]	53 Glycerol-2-phosphate	0.434
15908	64 [789; Tyramine (3TMS)]	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	0.370
7017	64 [789; Tyramine (3TMS)]	82 Lysine	0.370
7004	64 [789; Tyramine (3TMS)]	1 [938; Sulfuric acid (2TMS)]	0.381
6958	64 [789; Tyramine (3TMS)]	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	0.413
10006	64 [789; Tyramine (3TMS)]	107 [931; myo-Inositol-2-phosphate (7TMS)]	0.360
6969	64 [789; Tyramine (3TMS)]	119 [931; myo-Inositol-2-phosphate (7TMS)]	0.379
6971	64 [789; Tyramine (3TMS)]	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	0.379
6983	64 [789; Tyramine (3TMS)]	52 [NA]	0.357
6985	64 [789; Tyramine (3TMS)]	105 [705; 2-Ketogluconic acid (5TMS)]	0.413
6986	64 [789; Tyramine (3TMS)]		0.458
15820	64 [789; Tyramine (3TMS)]		0.458
6981	64 [789; Tyramine (3TMS)]		0.458



12476	64 [789; Tyramine (3TMS)]	20 [619; 2,4,3',4'-Bishydroxyphenyl]-2-oxoethylamine (4TMS)]	30 -0.448	-0.614	14.049	0.360	139	3	138	4	70	82 duplicate
6965	64 [789; Tyramine (3TMS)]	89 [775; Dopamine (4TMS)]	34 -0.458	-0.694	15.933	0.376	140	2	141	1	84	84 original
16806	64 [789; Tyramine (3TMS)]	63 Glutamine	61 -0.475	-0.650	15.516	0.406	141	1	139	3	82	56 duplicate
16324	65 [646; 3-Deoxyglucitol (5	57 [757; 2-Deoxy-pentos-3-ylose dimethoxyamine (2TMS)]	55 0.922	0.977	5.371	0.712	1	141	8	134	5	7 duplicate
15272	65 [646; 3-Deoxyglucitol (5	46 Arabinose	63 0.873	0.989	11.854	0.738	2	140	3	139	30	2 duplicate
11987	65 [646; 3-Deoxyglucitol (5	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	63 0.861	0.974	19.310	0.699	3	139	9	133	79	10 duplicate
12951	65 [646; 3-Deoxyglucitol (5	24 [725; 2-Ketooctanoic acid (2TMS)]	63 0.860	0.986	32.934	0.724	4	138	4	138	123	4 duplicate
7088	65 [646; 3-Deoxyglucitol (5	134 Isomaltose	63 0.850	0.993	22.503	0.734	5	137	1	141	94	3 original
7038	65 [646; 3-Deoxyglucitol (5	86 [793; D-Galactono-1,4-lactone (4TMS)]	60 0.847	0.979	16.081	0.715	6	136	5	137	56	8 original
16240	65 [646; 3-Deoxyglucitol (5	56 [829; Ornic acid (3TMS)]	63 0.847	0.989	3.737	0.740	7	135	2	140	2	1 duplicate
11609	65 [646; 3-Deoxyglucitol (5	13 Uracil	63 0.840	0.977	15.950	0.699	8	134	7	135	53	11 duplicate
15642	65 [646; 3-Deoxyglucitol (5	50 [746; Ribonic acid-1,4-lactone (3TMS)]	60 0.819	0.952	16.399	0.627	9	133	12	130	59	45 duplicate
7081	65 [646; 3-Deoxyglucitol (5	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59 0.806	0.977	3.095	0.685	10	132	6	136	1	16 original
12111	65 [646; 3-Deoxyglucitol (5	17 [700; 2-methyl-1,2-propanediol (2TMS)]	63 0.784	0.932	18.505	0.628	11	131	16	126	74	46 duplicate
7040	65 [646; 3-Deoxyglucitol (5	88 Gluconic acid	63 0.774	0.917	11.253	0.681	12	130	21	121	25	20 original
13521	65 [646; 3-Deoxyglucitol (5	29 Erythritol	63 0.768	0.942	11.698	0.652	13	129	13	129	29	32 duplicate
14586	65 [646; 3-Deoxyglucitol (5	39 [829; 1-Phenylethanol (1TMS)]	63 0.765	0.969	12.632	0.700	14	128	10	132	34	9 duplicate
15996	65 [646; 3-Deoxyglucitol (5	34 [NA]	54 0.755	0.942	8.156	0.628	15	127	14	126	14	44 duplicate
14484	65 [646; 3-Deoxyglucitol (5	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	63 0.744	0.961	11.499	0.667	16	126	11	131	27	26 duplicate
16729	65 [646; 3-Deoxyglucitol (5	62 [812; D-Xylofuranose (4TMS)]	63 0.729	0.935	17.669	0.676	17	125	15	127	69	22 duplicate
11352	65 [646; 3-Deoxyglucitol (5	11 Succinic acid	63 0.704	0.914	12.737	0.621	18	124	22	120	36	47 duplicate
7044	65 [646; 3-Deoxyglucitol (5	92 [880; Glycerol-2-phosphate (4TMS)]	53 0.678	0.807	6.437	0.618	19	123	37	105	9	50 original
7055	65 [646; 3-Deoxyglucitol (5	103 [648; Ethylamine (2TMS)]	62 0.676	0.829	10.761	0.565	20	122	36	106	23	70 original
7051	65 [646; 3-Deoxyglucitol (5	99 [682; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41 0.661	0.919	9.781	0.682	21	121	20	122	20	18 original
7057	65 [646; 3-Deoxyglucitol (5	105 [705; 2-Ketogluconic acid (5TMS)]	48 0.645	0.854	6.077	0.632	22	120	33	109	6	42 original
11736	65 [646; 3-Deoxyglucitol (5	14 Fumaric acid	63 0.631	0.822	11.359	0.668	23	119	18	124	26	25 duplicate
7025	65 [646; 3-Deoxyglucitol (5	73 [708; Glucose methoxyamine (5TMS)]	56 0.623	0.803	8.033	0.540	24	118	38	104	13	76 original
7049	65 [646; 3-Deoxyglucitol (5	97 [756; beta-D-Methylglucopyranoside (4TMS)]	52 0.621	0.800	15.441	0.568	25	117	39	103	48	67 original
11481	65 [646; 3-Deoxyglucitol (5	12 Glycic acid	62 0.617	0.855	12.044	0.610	26	116	32	110	32	56 duplicate
12716	65 [646; 3-Deoxyglucitol (5	22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52 0.602	0.807	9.888	0.613	27	115	23	119	19	53 duplicate
7028	65 [646; 3-Deoxyglucitol (5	76 Fructose	63 0.591	0.922	25.029	0.668	28	114	19	123	104	27 original
7022	65 [646; 3-Deoxyglucitol (5	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	56 0.590	0.646	21.532	0.521	29	113	58	84	89	83 original
13409	65 [646; 3-Deoxyglucitol (5	28 Malic acid	63 0.584	0.926	14.020	0.694	30	112	17	125	42	12 duplicate
7030	65 [646; 3-Deoxyglucitol (5	78 Mannose	61 0.580	0.858	7.568	0.595	31	111	29	113	10	59 original
7053	65 [646; 3-Deoxyglucitol (5	101 [832; Dopamine (4TMS)]	63 0.563	0.722	11.209	0.526	32	110	51	91	24	82 original
7077	65 [646; 3-Deoxyglucitol (5	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru	63 0.559	0.843	32.251	0.636	33	109	35	107	122	40 original
14687	65 [646; 3-Deoxyglucitol (5	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	63 0.558	0.857	37.475	0.647	34	108	30	112	132	35 duplicate
10007	65 [646; 3-Deoxyglucitol (5	1 [938; Sulfuric acid (2TMS)]	36 0.546	0.608	9.256	0.651	35	107	61	81	17	33 duplicate
7043	65 [646; 3-Deoxyglucitol (5	91 [768; beta-D-Methylglucopyranoside (4TMS)]	63 0.545	0.680	14.240	0.481	36	106	53	89	45	105 original
7058	65 [646; 3-Deoxyglucitol (5	106 [733; Threitol (4TMS)]	61 0.540	0.885	9.125	0.690	37	105	27	115	16	14 original
12597	65 [646; 3-Deoxyglucitol (5	11 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	63 0.529	0.763	20.111	0.569	38	104	44	98	82	65 duplicate
7087	65 [646; 3-Deoxyglucitol (5	115 Glucose-6-phosphate	61 0.520	0.892	25.524	0.672	39	103	26	116	107	23 original
7080	65 [646; 3-Deoxyglucitol (5	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45 0.517	0.867	4.033	0.642	40	102	28	114	3	37 original
14172	65 [646; 3-Deoxyglucitol (5	35 Pyroglutamic acid	63 0.490	0.896	43.247	0.665	41	101	25	117	138	28 duplicate
7072	65 [646; 3-Deoxyglucitol (5	120 [945; Uridine (3TMS)]	54 0.473	0.350	14.284	0.635	43	99	72	70	46	41 original
13182	65 [646; 3-Deoxyglucitol (5	28 Citramalic acid	63 0.472	0.771	20.981	0.535	44	98	43	99	84	80 duplicate
7039	65 [646; 3-Deoxyglucitol (5	87 [945; beta-D-Glucopyranose (5TMS)]	61 0.471	0.761	35.821	0.577	45	97	45	97	128	62 original
7073	65 [646; 3-Deoxyglucitol (5	121 [657; Erythritol (4TMS)]	54 0.442	0.761	12.894	0.614	46	96	46	96	38	51 original

7062	65 [646; 3-Deoxyglucitol (5' 110 [715; Erythritol (4TMS))]	54	0.431	0.844	7.803	0.882	47	95	34	108	12	17 original
7074	65 [646; 3-Deoxyglucitol (5' 122 [644; Erythritol (4TMS))]	52	0.427	0.858	12.874	0.809	48	94	31	111	37	57 original
10692	65 [646; 3-Deoxyglucitol (5' 6 Glycerol	63	0.424	0.739	44.082	0.566	49	93	49	93	140	69 duplicate
7069	65 [646; 3-Deoxyglucitol (5' 117 [724; Glycerol (3TMS))]	56	0.419	0.787	7.781	0.586	50	92	40	102	11	60 original
7052	65 [646; 3-Deoxyglucitol (5' 100 [657; Mannitol (6TMS))]	63	0.408	0.747	14.141	0.570	51	91	48	94	44	64 original
7054	65 [646; 3-Deoxyglucitol (5' 102 [904; Gelactose methoxamine (5TMS))]	63	0.398	0.678	12.312	0.544	52	90	54	88	33	74 original
7037	65 [646; 3-Deoxyglucitol (5' 85 [523; Methylcitric acid (4TMS))]	47	0.397	0.684	11.976	0.457	53	89	52	90	31	113 original
7064	65 [646; 3-Deoxyglucitol (5' 112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS))]	62	0.388	0.671	17.371	0.542	54	88	56	86	67	75 original
7084	65 [646; 3-Deoxyglucitol (5' 132 [895; Isomallose methoxamine (8TMS))]	42	0.354	0.902	12.939	0.845	55	87	24	118	39	36 original
15081	65 [646; 3-Deoxyglucitol (5' 44 [910; 2-Ketogluconic acid methoxamine (4TMS))]	50	0.344	0.785	6.395	0.632	56	86	41	101	7	43 duplicate
7087	65 [646; 3-Deoxyglucitol (5' 135 [902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS))]	63	0.326	0.553	18.050	0.499	57	85	64	78	71	84 original
7065	65 [646; 3-Deoxyglucitol (5' 113 Galactose-6-phosphate	61	0.317	0.781	9.442	0.584	58	84	42	100	18	61 original
12234	65 [646; 3-Deoxyglucitol (5' 18 [590; 1-Acetyl-2-thiohydantoin	63	0.297	0.537	14.108	0.443	59	83	65	77	43	121 duplicate
7079	65 [646; 3-Deoxyglucitol (5' 127 [777; Fructose-6-phosphate methoxamine (6TMS))]	39	0.293	0.727	6.409	0.679	60	82	50	92	8	21 original
7032	65 [646; 3-Deoxyglucitol (5' 80 [772; D-Glucose (5TMS))]	61	0.287	0.649	31.787	0.538	61	81	57	85	121	78 original
7026	65 [646; 3-Deoxyglucitol (5' 74 [912; Tetradecanoic acid (1TMS))]	63	0.253	0.585	11.846	0.461	62	80	63	79	28	112 original
7056	65 [646; 3-Deoxyglucitol (5' 104 [795; Erythritol (4TMS))]	62	0.252	0.512	12.645	0.537	63	79	66	76	35	79 original
7068	65 [646; 3-Deoxyglucitol (5' 116 [882; Pseudouridine (5TMS))]	30	0.237	0.348	10.394	0.494	64	78	73	68	22	96 duplicate
12356	65 [646; 3-Deoxyglucitol (5' 19 Alanine (BP) (3TMS)	63	0.228	0.641	15.461	0.569	65	77	59	83	49	66 duplicate
7066	65 [646; 3-Deoxyglucitol (5' 114 Fructose-6-phosphate	52	0.211	0.749	10.055	0.840	66	76	47	95	21	39 original
7036	65 [646; 3-Deoxyglucitol (5' 84 Mannitol	61	0.209	0.450	33.775	0.453	67	75	69	73	125	116 original
15366	65 [646; 3-Deoxyglucitol (5' 47 [NA]	63	0.208	0.203	16.012	0.491	68	74	81	61	54	101 duplicate
7078	65 [646; 3-Deoxyglucitol (5' 126 [559; Erythritol (4TMS))]	45	0.200	0.612	9.074	0.656	69	73	60	82	15	30 original
7048	65 [646; 3-Deoxyglucitol (5' 98 myo-Inositol	48	0.195	0.221	18.163	0.346	70	72	78	64	72	139 original
7045	65 [646; 3-Deoxyglucitol (5' 93 [607; Putrescine (4TMS))]	60	0.190	0.271	17.234	0.442	71	71	76	66	68	122 original
14787	65 [646; 3-Deoxyglucitol (5' 41 [639; Proline (2TMS))]	63	0.168	0.469	18.241	0.517	72	70	68	74	73	88 duplicate
7075	65 [646; 3-Deoxyglucitol (5' 123 [945; Galactofuranose-6-phosphate (7TMS))]	63	0.154	0.503	16.182	0.567	73	69	67	75	57	68 original
7035	65 [646; 3-Deoxyglucitol (5' 83 Sorbitol	57	0.140	-0.277	27.838	0.349	74	68	92	50	113	138 original
11862	65 [646; 3-Deoxyglucitol (5' 15 Alanine	63	0.094	0.373	22.249	0.690	75	67	70	72	92	13 duplicate
18884	65 [646; 3-Deoxyglucitol (5' 64 [789; Tyramine (3TMS))]	62	0.071	0.317	13.466	0.436	76	66	74	68	40	125 duplicate
7031	65 [646; 3-Deoxyglucitol (5' 79 Glucose	63	0.071	0.585	36.968	0.614	77	65	62	80	131	52 original
15909	65 [646; 3-Deoxyglucitol (5' 53 Glycerol-2-phosphate	63	0.060	-0.059	15.604	0.376	78	64	86	56	50	136 duplicate
7085	65 [646; 3-Deoxyglucitol (5' 133 [855; Squalene]	63	0.044	0.031	15.854	0.351	79	63	84	58	52	137 original
7092	65 [646; 3-Deoxyglucitol (5' 140 [692; Ergosta-7,22-dien-3-ol (1TMS))]	48	0.041	0.205	16.073	0.473	80	62	80	62	55	109 original
7063	65 [646; 3-Deoxyglucitol (5' 111 [583; Erythritol (4TMS))]	41	0.039	0.310	21.274	0.450	81	61	75	67	86	117 original
16807	65 [646; 3-Deoxyglucitol (5' 63 Glutamine	51	0.020	-0.756	26.078	0.724	82	60	122	20	110	5 duplicate
7042	65 [646; 3-Deoxyglucitol (5' 90 [910; 9-(Z)-Hexadecenoic acid (1TMS))]	63	0.013	-0.043	15.813	0.442	83	59	85	57	51	123 original
7061	65 [646; 3-Deoxyglucitol (5' 109 Octadecanoic acid	63	0.006	0.358	24.857	0.487	84	58	71	71	103	103 original
7070	65 [646; 3-Deoxyglucitol (5' 118 [928; Glucopyranose-6-phosphate (6TMS))]	58	-0.015	0.218	13.667	0.517	85	57	79	63	41	85 original
7093	65 [646; 3-Deoxyglucitol (5' 141 Lanosta-8,24-dien-3-beta-ol	60	-0.049	0.064	16.298	0.491	86	56	82	60	58	89 original
7046	65 [646; 3-Deoxyglucitol (5' 94 Hexadecanoic acid	63	-0.063	0.263	25.312	0.487	87	55	77	65	106	102 original
7091	65 [646; 3-Deoxyglucitol (5' 139 [700; Ergosta-5,7-dien-3-ol]	37	-0.072	-0.153	19.093	0.502	88	54	87	55	78	93 original
7024	65 [646; 3-Deoxyglucitol (5' 72 [919; D-Xylopyranose (4TMS))]	62	-0.082	-0.183	16.943	0.379	89	53	90	52	64	135 original
7090	65 [646; 3-Deoxyglucitol (5' 138 [674; Ergosterol (1TMS))]	46	-0.136	0.043	18.016	0.486	90	52	83	59	70	104 original
7059	65 [646; 3-Deoxyglucitol (5' 107 9-(Z)-Octadecenoic acid	63	-0.141	-0.287	21.098	0.440	91	51	93	49	85	124 original
7071	65 [646; 3-Deoxyglucitol (5' 119 [931; myo-Inositol-2-phosphate (7TMS))]	63	-0.147	-0.168	17.009	0.518	92	50	88	54	65	84 original
14984	65 [646; 3-Deoxyglucitol (5' 43 [548; Leucine (2TBS))]	59	-0.149	-0.394	17.499	0.506	93	49	96	46	68	91 duplicate
7089	65 [646; 3-Deoxyglucitol (5' 137 Ergosterol	63	-0.154	-0.179	21.541	0.467	94	48	89	53	90	111 original
15821	65 [646; 3-Deoxyglucitol (5' 52 [NA]	45	-0.166	-0.665	25.270	0.668	95	47	114	28	105	24 duplicate
7023	65 [646; 3-Deoxyglucitol (5' 71 [731; Erythrose (3TMS))]	63	-0.188	-0.242	19.056	0.444	96	46	91	51	77	119 original

10421	65 [646; 3-Deoxyglucitol (5' 124 [734; 1-Monocleoylglycerol (2TMS); 1-Phosphoric acid	50 -0.207	-0.397	38.931	0.281	97	45	97	45	136	141 duplicate
7076	65 [646; 3-Deoxyglucitol (5' 130 Monohexadecanoylglycerol (1TMS))	58 -0.228	-0.330	24.265	0.443	98	44	95	47	102	120 original
7082	65 [646; 3-Deoxyglucitol (5' 130 Trehalose	62 -0.261	-0.301	33.644	0.385	99	43	94	48	124	133 original
13067	65 [646; 3-Deoxyglucitol (5' 25 [709; 2,5-Diaminovalerolactam (2TMS))	48 -0.266	-0.909	23.234	0.656	100	42	137	5	96	31 duplicate
7020	65 [646; 3-Deoxyglucitol (5' 68 [570; Hypoxanthine (2TMS))	20 -0.274	-0.916	15.338	0.619	101	41	138	4	47	48 original
16650	65 [646; 3-Deoxyglucitol (5' 61 [NA]	63 -0.283	-0.460	16.438	0.508	102	40	100	42	60	90 duplicate
7088	65 [646; 3-Deoxyglucitol (5' 138 [748; D-Sedoheptulose-7-phosphate (7TMS))	17 -0.294	-0.454	5.371	0.539	103	39	99	43	4	77 original
7050	65 [646; 3-Deoxyglucitol (5' 98 [697; Ribose-5-phosphate methoxyamine (5TMS))	47 -0.308	-0.784	22.150	0.531	104	38	123	19	91	81 original
7060	65 [646; 3-Deoxyglucitol (5' 108 Octadecenoic acid	63 -0.319	-0.486	16.931	0.402	105	37	101	41	63	132 original
16407	65 [646; 3-Deoxyglucitol (5' 58 [636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS))	63 -0.341	-0.420	23.752	0.383	106	36	98	44	99	134 duplicate
13296	65 [646; 3-Deoxyglucitol (5' 27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS))	52 -0.360	-0.804	25.688	0.557	107	35	124	18	108	72 duplicate
7041	65 [646; 3-Deoxyglucitol (5' 89 [775; Dopamine (4TMS))	34 -0.387	-0.867	24.007	0.612	108	34	134	8	100	55 original
7027	65 [646; 3-Deoxyglucitol (5' 75 Lysine	63 -0.390	-0.524	43.879	0.436	109	33	102	40	139	126 original
12834	65 [646; 3-Deoxyglucitol (5' 23 Homoserine	63 -0.392	-0.832	22.801	0.618	110	32	129	13	95	49 duplicate
15551	65 [646; 3-Deoxyglucitol (5' 49 [877; Pyrophosphoric acid (4TMS))	63 -0.395	-0.808	25.972	0.455	111	31	107	35	109	114 duplicate
14277	65 [646; 3-Deoxyglucitol (5' 38 [596; N-Acetylglutamic acid (2TMS))	63 -0.402	-0.565	34.305	0.426	112	30	105	37	126	128 duplicate
15177	65 [646; 3-Deoxyglucitol (5' 45 Homocysteine	60 -0.425	-0.620	23.451	0.447	113	29	108	34	98	118 duplicate
10826	65 [646; 3-Deoxyglucitol (5' 7 Threonine	63 -0.439	-0.546	34.814	0.408	114	28	104	38	127	131 duplicate
7018	65 [646; 3-Deoxyglucitol (5' 66 Glycine acid-3-phosphate	63 -0.454	-0.626	16.516	0.472	115	27	110	32	61	110 original
7047	65 [646; 3-Deoxyglucitol (5' 85 [770; 3,4,6-Trisubstituted phenylethanolamine (5TMS))	49 -0.459	-0.689	21.384	0.492	116	26	115	27	87	97 original
10146	65 [646; 3-Deoxyglucitol (5' 2 Serine	61 -0.472	-0.608	28.597	0.421	117	25	106	36	118	129 duplicate
7083	65 [646; 3-Deoxyglucitol (5' 131 [626; 5-Methylthiadenosine (3TMS))	54 -0.480	-0.716	19.954	0.575	118	24	119	23	80	63 original
13742	65 [646; 3-Deoxyglucitol (5' 31 [622; Parabanic acid (2TMS))	63 -0.492	-0.714	18.743	0.564	119	23	118	24	75	71 duplicate
10959	65 [646; 3-Deoxyglucitol (5' 8 Isoleucine	54 -0.497	-0.542	27.843	0.323	120	22	103	39	115	140 duplicate
7019	65 [646; 3-Deoxyglucitol (5' 67 Citric acid	63 -0.509	-0.639	28.901	0.476	121	21	111	31	119	108 original
16570	65 [646; 3-Deoxyglucitol (5' 60 Glycerol-3-phosphate	63 -0.515	-0.620	27.593	0.513	122	20	109	33	112	87 duplicate
15459	65 [646; 3-Deoxyglucitol (5' 48 Asparagine	63 -0.517	-0.658	24.048	0.682	123	19	133	9	101	19 duplicate
14066	65 [646; 3-Deoxyglucitol (5' 34 Aspartic acid	63 -0.525	-0.648	38.420	0.496	124	18	112	30	134	95 duplicate
14381	65 [646; 3-Deoxyglucitol (5' 37 Phenylalanine	63 -0.538	-0.709	28.404	0.512	125	17	116	26	117	88 duplicate
15732	65 [646; 3-Deoxyglucitol (5' 51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS))	43 -0.557	-0.814	20.072	0.492	126	16	126	16	81	98 duplicate
13959	65 [646; 3-Deoxyglucitol (5' 33 Methionine	63 -0.566	-0.712	22.337	0.509	127	15	117	25	93	89 duplicate
11091	65 [646; 3-Deoxyglucitol (5' 9 Proline	62 -0.567	-0.659	36.109	0.420	128	14	113	29	129	130 duplicate
16082	65 [646; 3-Deoxyglucitol (5' 55 [612; 4-Aminobutyric acid (2TBS))	42 -0.577	-0.851	21.425	0.545	129	13	132	10	88	73 duplicate
13632	65 [646; 3-Deoxyglucitol (5' 30 [815; Ethyl-3-(2H)-thiophenone]	63 -0.619	-0.719	36.880	0.429	130	12	120	22	130	127 duplicate
10557	65 [646; 3-Deoxyglucitol (5' 5 Leucine	44 -0.628	-0.818	18.832	0.503	131	11	127	15	76	92 duplicate
7021	65 [646; 3-Deoxyglucitol (5' 69 Arginine	59 -0.654	-0.903	31.213	0.640	132	10	136	6	120	38 original
10284	65 [646; 3-Deoxyglucitol (5' 3 Ethanolamine	61 -0.660	-0.849	20.363	0.605	133	9	131	11	83	58 duplicate
13851	65 [646; 3-Deoxyglucitol (5' 32 [729; N,N-Dimethyllysine methyl ester]	62 -0.665	-0.840	26.454	0.613	134	8	130	12	111	54 duplicate
16489	65 [646; 3-Deoxyglucitol (5' 59 Ornithine; Arginine	63 -0.671	-0.732	45.486	0.491	135	7	121	21	141	100 duplicate
12477	65 [646; 3-Deoxyglucitol (5' 20 [619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	30 -0.678	-0.941	16.845	0.647	136	6	139	3	62	34 duplicate
7029	65 [646; 3-Deoxyglucitol (5' 77 [626; beta-[(5-methyl-2-thienyl)methyl]amino-benzeneacetic acid methyl ester]	61 -0.702	-0.825	38.015	0.476	137	5	128	14	133	107 original
7034	65 [646; 3-Deoxyglucitol (5' 82 Lysine	38 -0.713	-0.987	27.708	0.689	138	4	141	1	114	15 original
11222	65 [646; 3-Deoxyglucitol (5' 10 Glycine	63 -0.731	-0.961	28.200	0.711	139	3	140	2	116	8 duplicate
14886	65 [646; 3-Deoxyglucitol (5' 42 Glutamic acid	59 -0.735	-0.810	38.780	0.478	140	2	125	17	135	106 duplicate
7033	65 [646; 3-Deoxyglucitol (5' 81 Tyrosine	63 -0.753	-0.900	41.020	0.657	141	1	135	7	137	29 original
10147	66 Glycine acid-3-phospho 2 Serine	62 0.621	0.770	17.662	0.487	1	141	5	137	96	49 duplicate
11092	66 Glycine acid-3-phospho 9 Proline	63 0.617	0.791	26.922	0.486	2	140	3	139	119	39 duplicate

13743	66	Glycine acid-3-phospho	31	[622; Parabenic acid (2TMS)]	64	0.613	0.761	5.629	0.532	3	139	7	135	7	13 duplicate
12835	66	Glycine acid-3-phospho	27	Homoserine	64	0.568	0.687	8.687	0.496	4	138	16	126	25	40 duplicate
13297	66	Glycine acid-3-phospho	23	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	0.559	0.739	14.988	0.493	5	137	11	131	75	43 duplicate
10950	66	Glycine acid-3-phospho	8	Isoleucine	55	0.546	0.721	17.338	0.514	6	136	14	128	92	28 duplicate
10827	66	Glycine acid-3-phospho	7	Threonine	64	0.539	0.763	30.760	0.473	7	135	6	136	127	61 duplicate
7108	66	Glycine acid-3-phospho	81	Tyrosine	64	0.527	0.758	34.181	0.528	8	134	8	134	134	16 original
13852	66	Glycine acid-3-phospho	32	[728; N,N-Dimethyllysine methyl ester]	63	0.526	0.776	11.757	0.540	9	133	4	138	47	11 duplicate
16490	66	Glycine acid-3-phospho	59	Ornithine; Arginine	64	0.500	0.740	41.579	0.455	10	132	9	133	139	78 duplicate
13633	66	Glycine acid-3-phospho	30	[815; Ethyl-3-(2H)-thiophenone]	64	0.496	0.641	29.999	0.395	11	130	23	119	125	115 duplicate
13960	66	Glycine acid-3-phospho	33	Methionine	64	0.496	0.544	9.228	0.440	12	131	30	112	29	83 duplicate
7102	66	Glycine acid-3-phospho	75	Lysine	64	0.492	0.794	40.304	0.482	13	129	2	140	138	54 original
7125	66	Glycine acid-3-phospho	98	[897; Ribose-5-phosphate methoxyamine (5TMS)]	48	0.482	0.638	14.714	0.495	14	128	24	118	72	41 original
14278	66	Glycine acid-3-phospho	36	[596; N-Acetylglutamic acid (2TMS)]	64	0.481	0.837	28.884	0.515	15	127	1	141	122	27 duplicate
11223	66	Glycine acid-3-phospho	10	Glycine	64	0.478	0.686	18.728	0.524	16	126	17	125	98	17 duplicate
10285	66	Glycine acid-3-phospho	3	Ethanolamine	62	0.476	0.873	6.728	0.461	17	125	19	123	9	72 duplicate
7095	66	Glycine acid-3-phospho	68	[570; Hypoxanthine (2TMS)]	20	0.453	0.586	12.302	0.462	18	124	29	113	51	71 original
14382	66	Glycine acid-3-phospho	37	Phenylalanine	64	0.451	0.729	23.159	0.473	19	123	12	130	113	62 duplicate
14067	66	Glycine acid-3-phospho	34	Aspartic acid	64	0.443	0.543	33.286	0.392	20	122	31	111	130	118 duplicate
16408	66	Glycine acid-3-phospho	58	[636; 4R-Acetalamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	0.439	0.739	15.604	0.471	21	121	10	132	80	65 duplicate
7096	66	Glycine acid-3-phospho	69	Arginine	60	0.429	0.659	20.565	0.516	22	120	22	120	108	25 original
7104	66	Glycine acid-3-phospho	67	[826; beta-[[[5-methyl-2-thienyl)methyl]ureaamino-benzeneacetic acid methyl ester]	62	0.424	0.722	29.486	0.506	23	119	13	129	124	35 original
7094	66	Glycine acid-3-phospho	42	Citric acid	64	0.397	0.695	24.314	0.440	24	118	15	127	116	95 original
14887	66	Glycine acid-3-phospho	42	Glutamic acid	60	0.394	0.682	29.124	0.467	25	117	18	124	123	67 duplicate
16571	66	Glycine acid-3-phospho	60	Glycerol-3-phosphate	64	0.379	0.663	21.723	0.511	26	116	21	121	111	30 duplicate
15178	66	Glycine acid-3-phospho	45	Homocysteine	61	0.345	0.321	17.257	0.459	27	115	38	104	91	73 duplicate
15460	66	Glycine acid-3-phospho	48	Asparagine	64	0.339	0.488	10.135	0.475	28	114	33	109	35	60 duplicate
7116	66	Glycine acid-3-phospho	51	[775; Dopamine (4TMS)]	35	0.334	0.353	14.131	0.438	29	113	35	107	66	97 original
15733	66	Glycine acid-3-phospho	59	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	0.328	0.615	16.419	0.508	30	112	27	115	87	33 duplicate
7157	66	Glycine acid-3-phospho	130	Trehalose	63	0.327	0.502	30.615	0.410	31	111	32	110	126	108 original
13088	66	Glycine acid-3-phospho	25	[708; 2,5-Diaminovalerolactam (2TMS)]	48	0.309	0.632	11.451	0.513	32	110	25	117	44	29 duplicate
10558	66	Glycine acid-3-phospho	5	Leucine	45	0.285	0.488	8.396	0.574	33	109	34	108	21	3 duplicate
7098	66	Glycine acid-3-phospho	71	[731; Erythrose (3TMS)]	64	0.265	0.602	11.934	0.471	34	108	28	114	48	64 original
7110	66	Glycine acid-3-phospho	83	Sorbitol	58	0.263	0.666	20.448	0.530	35	107	20	122	106	15 original
14985	66	Glycine acid-3-phospho	43	[548; Leucine (2TMS)]	60	0.246	0.250	7.148	0.383	36	106	45	97	11	121 duplicate
16885	66	Glycine acid-3-phospho	64	[789; Tyramine (3TMS)]	63	0.241	0.238	3.867	0.331	37	105	46	96	3	139 duplicate
7109	66	Glycine acid-3-phospho	82	Lysine	39	0.233	0.331	15.886	0.535	38	104	37	105	82	12 original
16651	66	Glycine acid-3-phospho	61	[NA]	64	0.222	0.254	5.163	0.346	39	103	44	98	5	134 duplicate
16083	66	Glycine acid-3-phospho	55	[612; 4-Aminobutyric acid (2TBS)]	43	0.212	0.209	19.564	0.487	40	102	49	93	105	50 duplicate
7158	66	Glycine acid-3-phospho	131	[626; 5-Methyladenosine (3TMS)]	55	0.211	0.271	12.478	0.453	41	101	39	103	54	81 original
10422	66	Glycine acid-3-phospho	4	Phosphoric acid	51	0.197	0.619	32.775	0.480	42	100	26	116	129	57 duplicate
7108	66	Glycine acid-3-phospho	79	Glucose	64	0.194	0.018	35.987	0.492	43	99	59	83	136	45 original
15552	66	Glycine acid-3-phospho	49	[877; Pyrophosphoric acid (4TMS)]	64	0.156	0.148	16.756	0.364	44	98	53	89	89	126 duplicate
11863	66	Glycine acid-3-phospho	15	Alanine	64	0.154	0.167	19.025	0.450	45	97	51	91	99	83 duplicate
7122	66	Glycine acid-3-phospho	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	0.153	0.236	15.985	0.361	46	96	47	95	84	127 original
7135	66	Glycine acid-3-phospho	108	Octadecenoic acid	64	0.134	0.332	4.777	0.371	47	95	36	106	4	124 original
16808	66	Glycine acid-3-phospho	63	Glutamine	52	0.095	0.265	13.643	0.398	48	94	42	100	65	113 duplicate
7131	66	Glycine acid-3-phospho	104	[795; Erythritol (4TMS)]	63	0.075	0.148	7.456	0.444	49	93	52	90	13	89 original
7150	66	Glycine acid-3-phospho	123	[945; Galactofuranose-6-phosphate (7TMS)]	64	0.060	0.134	10.955	0.516	50	92	54	88	41	24 original
15822	66	Glycine acid-3-phospho	52	[NA]	46	0.051	0.120	16.219	0.507	51	91	55	87	86	34 duplicate

7151	66 Glyceral acid-3-phosphate	124 [734; 1-Monocleoylglycerol (2TMS); 1-Monohexadecenoyleglycerol (1TMS)]	59	0.044	0.266	18.138	0.351	52	80	41	101	101	132 original
7160	66 Glyceral acid-3-phosphate	133 [855; Squalene]	64	0.040	0.268	7.264	0.411	53	89	40	102	12	107 original
7140	66 Glyceral acid-3-phosphate	113 Galactose-6-phosphate	62	-0.002	-0.145	8.503	0.485	54	88	69	73	23	68 original
7141	66 Glyceral acid-3-phosphate	114 Fructose-6-phosphate	53	-0.013	-0.161	7.763	0.524	55	87	73	69	16	18 original
7165	66 Glyceral acid-3-phosphate	138 [674; Ergosterol (1TMS)]	46	-0.016	0.258	12.029	0.488	56	86	43	99	49	48 original
7164	66 Glyceral acid-3-phosphate	137 Ergosterol	64	-0.033	0.228	14.512	0.395	57	85	48	94	70	118 original
7145	66 Glyceral acid-3-phosphate	118 [928; Glucopyranose-6-phosphate (6TMS)]	58	-0.038	-0.091	8.447	0.338	58	84	64	78	22	138 original
7138	66 Glyceral acid-3-phosphate	111 [583; Erythritol (4TMS)]	42	-0.050	0.014	15.788	0.355	59	83	60	82	81	130 original
7163	66 Glyceral acid-3-phosphate	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.059	0.203	3.837	0.448	60	82	50	92	2	87 original
14788	66 Glyceral acid-3-phosphate	41 [639; Proline (2TMS)]	64	-0.078	-0.076	14.316	0.438	61	81	63	79	68	98 duplicate
7136	66 Glyceral acid-3-phosphate	109 Octadecanoic acid	64	-0.081	0.081	23.329	0.415	62	80	58	84	114	105 original
12357	66 Glyceral acid-3-phosphate	19 Alanine (BP) (3TMS)	64	-0.083	-0.118	12.813	0.450	63	79	68	74	59	85 duplicate
7099	66 Glyceral acid-3-phosphate	72 [919; D-Xylopyranose (4TMS)]	63	-0.086	-0.111	8.304	0.343	64	78	65	77	20	138 original
7121	66 Glyceral acid-3-phosphate	94 Hexadecanoic acid	64	-0.086	0.085	22.434	0.439	65	77	57	85	112	96 original
12478	66 Glyceral acid-3-phosphate	20 [619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.097	0.108	13.415	0.544	66	76	56	86	62	8 duplicate
12235	66 Glyceral acid-3-phosphate	18 [590; 1-Acetyl-2-thiohydantoin]	67	-0.105	-0.117	7.981	0.382	67	75	67	75	18	122 duplicate
7100	66 Glyceral acid-3-phosphate	73 [708; Glucose methoxyamine (5TMS)]	57	-0.109	-0.160	10.727	0.411	68	74	72	70	38	106 original
7146	66 Glyceral acid-3-phosphate	119 [931; myo-Inositol-2-phosphate (7TMS)]	64	-0.113	-0.150	8.759	0.341	69	73	70	72	27	137 original
7153	66 Glyceral acid-3-phosphate	126 [559; Erythritol (4TMS)]	45	-0.115	-0.115	8.160	0.585	70	72	66	76	19	1 original
15910	66 Glyceral acid-3-phosphate	53 Glycerol-2-phosphate	64	-0.121	-0.200	7.472	0.324	71	71	78	64	14	141 duplicate
7134	66 Glyceral acid-3-phosphate	107 9-(Z)-Octadecanoic acid	64	-0.125	-0.024	15.020	0.346	72	69	81	81	76	133 original
10893	66 Glyceral acid-3-phosphate	6 Glycerol	64	-0.125	-0.253	42.913	0.369	73	70	81	61	141	125 duplicate
7166	66 Glyceral acid-3-phosphate	139 [700; Ergosta-5,7-dien-3-ol]	38	-0.129	-0.177	14.228	0.325	74	68	74	68	67	140 original
7168	66 Glyceral acid-3-phosphate	141 Lanosta-8,24-dien-3-beta-ol	61	-0.145	-0.066	10.871	0.443	75	67	62	80	39	90 original
14173	66 Glyceral acid-3-phosphate	35 Pyrogulamic acid	64	-0.156	-0.316	42.492	0.397	76	66	88	54	140	114 duplicate
7148	66 Glyceral acid-3-phosphate	121 [657; Erythritol (4TMS)]	55	-0.157	-0.194	11.580	0.442	77	65	77	65	45	91 original
7152	66 Glyceral acid-3-phosphate	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	-0.171	-0.311	33.450	0.372	78	64	88	56	131	123 original
7123	66 Glyceral acid-3-phosphate	96 myo-Inositol	49	-0.179	-0.158	15.961	0.357	79	63	71	83	128	original
7105	66 Glyceral acid-3-phosphate	78 Mannose	62	-0.187	-0.317	11.730	0.399	80	62	90	52	46	111 original
15082	66 Glyceral acid-3-phosphate	44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	-0.195	-0.252	12.073	0.522	81	61	80	82	50	19 duplicate
7142	66 Glyceral acid-3-phosphate	115 Glucose-6-phosphate	62	-0.195	-0.321	26.031	0.433	82	59	91	51	118	100 original
7107	66 Glyceral acid-3-phosphate	80 [772; D-Glucose (5TMS)]	62	-0.195	-0.340	32.175	0.356	83	60	93	49	128	129 original
14888	66 Glyceral acid-3-phosphate	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.195	-0.345	35.476	0.518	84	58	94	48	135	23 duplicate
7149	66 Glyceral acid-3-phosphate	122 [644; Erythritol (4TMS)]	52	-0.196	-0.379	14.461	0.510	85	57	99	43	69	31 original
7147	66 Glyceral acid-3-phosphate	120 [945; Uridine (3TMS)]	54	-0.203	-0.182	12.890	0.560	86	56	75	67	80	8 original
7103	66 Glyceral acid-3-phosphate	76 Fructose	64	-0.207	-0.366	27.301	0.435	87	55	96	46	120	99 original
7129	66 Glyceral acid-3-phosphate	102 [904; Galactose methoxyamine (5TMS)]	64	-0.208	-0.268	5.182	0.416	88	54	83	59	6	104 original
7112	66 Glyceral acid-3-phosphate	85 [529; Methylcitric acid (4TMS)]	48	-0.211	-0.266	2.957	0.576	89	53	82	60	1	2 original
7101	66 Glyceral acid-3-phosphate	74 [912; Erythritol (4TMS)]	54	-0.216	-0.312	12.781	0.550	90	52	87	55	58	7 original
7133	66 Glyceral acid-3-phosphate	106 [733; Threitol (4TMS)]	64	-0.235	-0.191	10.885	0.457	91	51	76	66	40	75 original
7144	66 Glyceral acid-3-phosphate	117 [724; Glycerol (3TMS)]	62	-0.236	-0.337	12.953	0.566	92	50	92	50	61	5 original
7127	66 Glyceral acid-3-phosphate	100 [857; Mannitol (6TMS)]	56	-0.243	-0.347	10.029	0.520	93	49	95	47	33	20 original
7097	66 Glyceral acid-3-phosphate	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	64	-0.246	-0.399	9.508	0.444	94	48	101	41	31	88 original
13410	66 Glyceral acid-3-phosphate	28 Malic acid	57	-0.247	-0.249	19.120	0.387	95	47	79	63	100	120 original
12598	66 Glyceral acid-3-phosphate	21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	-0.249	-0.552	10.088	0.490	96	46	112	30	34	47 duplicate
135	66 Glyceral acid-3-phosphate	135	64	-0.250	-0.443	17.554	0.449	97	45	105	37	84	86 duplicate
7162	66 Glyceral acid-3-phosphate	135	64	-0.259	-0.275	12.510	0.428	98	44	85	57	55	102 original
7117	66 Glyceral acid-3-phosphate	80 [902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	-0.262	-0.317	7.948	0.345	99	43	89	53	17	135 original

7167	66 Glycemic acid-3-phospho	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	49	-0.264	-0.273	12.313	0.440	100	42	84	58	52	92 original
13183	66 Glycemic acid-3-phospho	26	Citramalic acid	64	-0.267	-0.428	16.956	0.428	101	41	104	38	90	103 duplicate
14485	66 Glycemic acid-3-phospho	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.286	-0.618	9.250	0.531	102	40	117	25	30	14 duplicate
7154	66 Glycemic acid-3-phospho	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	39	-0.301	-0.513	7.536	0.394	104	38	107	35	15	117 original
7159	66 Glycemic acid-3-phospho	132	[895; Isomaltose methoxyamine (6TMS)]	42	-0.303	-0.638	15.192	0.481	105	37	122	20	78	56 original
7139	66 Glycemic acid-3-phospho	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	-0.306	-0.379	12.673	0.506	106	36	98	44	57	36 original
11737	66 Glycemic acid-3-phospho	14	Fumaric acid	64	-0.322	-0.588	7.146	0.477	107	35	113	29	10	58 duplicate
7111	66 Glycemic acid-3-phospho	84	Mannitol	62	-0.323	-0.778	33.666	0.542	108	34	139	3	132	10 original
15367	66 Glycemic acid-3-phospho	47	[NA]	64	-0.325	-0.523	12.541	0.455	109	33	109	33	56	80 duplicate
7114	66 Glycemic acid-3-phospho	87	[945; beta-D-Glucopyranose (5TMS)]	62	-0.335	-0.418	36.675	0.398	110	32	103	39	137	112 original
11353	66 Glycemic acid-3-phospho	91	Succinic acid	64	-0.338	-0.544	8.710	0.463	111	31	111	31	26	70 duplicate
7120	66 Glycemic acid-3-phospho	93	[807; Putrescine (4TMS)]	60	-0.339	-0.617	14.668	0.451	112	30	116	28	71	82 original
13522	66 Glycemic acid-3-phospho	29	Erythritol	64	-0.355	-0.845	6.076	0.519	113	29	123	19	8	22 duplicate
7113	66 Glycemic acid-3-phospho	86	[793; D-Galactono-1,4-lactone (4TMS)]	61	-0.360	-0.519	24.626	0.510	114	28	108	34	117	32 original
7128	66 Glycemic acid-3-phospho	101	[832; Dopamine (4TMS)]	64	-0.362	-0.705	13.636	0.456	115	27	132	10	64	76 original
16730	66 Glycemic acid-3-phospho	62	[812; D-Xylofuranose (4TMS)]	64	-0.363	-0.536	15.056	0.450	116	26	110	32	77	84 duplicate
7155	66 Glycemic acid-3-phospho	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	-0.366	-0.473	10.964	0.391	117	25	106	36	42	119 original
12952	66 Glycemic acid-3-phospho	24	[725; 2-Ketocanoic acid (2TMS)]	64	-0.366	-0.659	33.732	0.488	118	24	126	16	133	52 duplicate
7118	66 Glycemic acid-3-phospho	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	-0.394	-0.764	20.494	0.493	119	23	138	4	107	42 original
11988	66 Glycemic acid-3-phospho	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	-0.398	-0.677	19.469	0.516	120	22	129	13	103	26 duplicate
14587	66 Glycemic acid-3-phospho	39	[829; 1-Phenylethanol (1TMS)]	63	-0.398	-0.664	19.335	0.486	121	21	127	15	102	51 duplicate
11482	66 Glycemic acid-3-phospho	12	Glycemic acid	63	-0.403	-0.625	8.840	0.456	122	20	118	24	28	77 duplicate
12112	66 Glycemic acid-3-phospho	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	-0.409	-0.613	19.466	0.458	123	19	115	27	104	74 duplicate
7115	66 Glycemic acid-3-phospho	88	Gluconic acid	64	-0.411	-0.674	14.789	0.483	124	18	128	14	73	53 original
7130	66 Glycemic acid-3-phospho	103	[648; Ethylamine (2TMS)]	63	-0.428	-0.744	17.634	0.503	125	17	136	6	95	38 original
16241	66 Glycemic acid-3-phospho	56	[829; Ornic acid (3TMS)]	64	-0.429	-0.628	13.552	0.464	126	16	120	22	63	69 duplicate
12717	66 Glycemic acid-3-phospho	22	[690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	52	-0.436	-0.702	11.202	0.543	127	15	131	11	43	9 duplicate
7161	66 Glycemic acid-3-phospho	134	Isomaltose	64	-0.453	-0.650	27.752	0.476	128	14	124	18	121	59 original
16961	66 Glycemic acid-3-phospho	65	[646; 3-Deoxyglucitol (5TMS)]	63	-0.454	-0.626	16.516	0.472	129	13	119	23	88	63 duplicate
15273	66 Glycemic acid-3-phospho	46	Arabinose	64	-0.456	-0.611	20.789	0.471	130	12	114	28	109	66 duplicate
7143	66 Glycemic acid-3-phospho	116	[882; Pseudouridine (5TMS)]	30	-0.457	-0.371	8.624	0.455	131	11	97	45	24	79 original
15997	66 Glycemic acid-3-phospho	54	[NA]	55	-0.479	-0.629	12.400	0.404	132	10	121	21	53	110 duplicate
7119	66 Glycemic acid-3-phospho	92	[680; Glycerol-2-phosphate (4TMS)]	54	-0.488	-0.415	10.682	0.353	133	9	102	40	37	131 original
15643	66 Glycemic acid-3-phospho	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	-0.501	-0.712	16.001	0.493	134	8	134	8	85	44 duplicate
11610	66 Glycemic acid-3-phospho	13	Uracil	64	-0.501	-0.715	18.573	0.519	135	7	135	7	97	21 duplicate
7126	66 Glycemic acid-3-phospho	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	-0.534	-0.707	10.322	0.429	136	6	133	9	36	101 original
7124	66 Glycemic acid-3-phospho	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	-0.538	-0.746	24.213	0.503	137	5	137	5	115	37 original
7156	66 Glycemic acid-3-phospho	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	59	-0.545	-0.696	14.942	0.491	138	4	130	12	74	46 original
16325	66 Glycemic acid-3-phospho	57	[757; 2-Desoxy-pentose-3-ylose dimethoxyamine (2TMS)]	55	-0.548	-0.658	17.446	0.481	139	3	125	17	93	55 duplicate
10008	66 Glycemic acid-3-phospho	1	[938; Sulfuric acid (2TMS)]	36	-0.559	-0.808	9.851	0.569	140	2	141	1	32	4 duplicate
7132	66 Glycemic acid-3-phospho	105	[705; 2-Ketogluconic acid (5TMS)]	48	-0.612	-0.802	15.568	0.440	141	1	140	2	79	94 original
16572	67 Clitic acid	60	Glycerol-3-phosphate	64	0.714	0.895	3.687	0.591	1	141	1	141	2	3 duplicate
14333	67 Clitic acid	37	Phenylalanine	64	0.695	0.836	2.011	0.533	2	140	5	137	1	10 duplicate
10286	67 Clitic acid	3	Ethanolamine	62	0.692	0.842	28.515	0.540	3	139	4	138	111	8 duplicate
7182	67 Clitic acid	81	Tyrosine	64	0.691	0.879	12.726	0.535	4	138	2	140	31	9 original
7178	67 Clitic acid	77	[826; beta-[[[5-methyl-2-thienyl)methylethylamino]-benzeneacetic acid methyl ester]	62	0.671	0.850	12.151	0.468	5	137	3	139	23	28 original
7172	67 Clitic acid	71	[731; Erythrose (3TMS)]	64	0.592	0.809	12.636	0.507	6	136	6	136	29	17 original
16084	67 Clitic acid	55	[612; 4-Aminobutyric acid (2TBS)]	43	0.550	0.749	37.594	0.521	7	135	9	133	136	13 duplicate

[illegible]

7231	67 Citric acid	130 Trehalose	63	0,118	0,286	7,161	0,378	57	85	54	88	4	108 original
16409	67 Citric acid	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	58	0,094	0,593	11,513	0,428	58	84	25	117	20	65 duplicate
7186	67 Citric acid	[528; Methylenic acid (4TMS)]	85	0,094	0,139	19,904	0,475	59	83	61	81	68	27 original
7181	67 Citric acid	[910; 9-(Z)-Hexadecanoic acid (1TMS)]	116	0,083	0,050	19,868	0,397	60	82	65	77	67	98 original
7217	67 Citric acid	[882; Pseudouridine (5TMS)]	135	0,071	0,434	20,054	0,465	61	81	39	103	69	30 original
7236	67 Citric acid	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	25	0,068	0,123	12,613	0,390	62	80	63	79	28	102 original
13069	67 Citric acid	[709; 2,5-Diaminovalerolactam (2TMS)]	44	0,055	0,278	26,965	0,360	63	79	55	87	105	124 duplicate
15083	67 Citric acid	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	113	0,051	0,016	18,647	0,384	64	78	66	76	57	105 duplicate
7214	67 Citric acid	Galactose-6-phosphate	62	0,050	-0,369	28,208	0,553	65	77	95	47	101	4 original
7215	67 Citric acid	Fructose-6-phosphate	74	0,012	-0,288	25,344	0,510	66	76	87	55	96	16 original
16886	67 Citric acid	[912; Tetradecanoic acid (1TMS)]	64	0,011	0,057	25,534	0,399	67	76	64	78	88	92 original
7224	67 Citric acid	[789; Tyramine (3TMS)]	63	-0,001	-0,057	22,781	0,397	68	74	71	84	95 duplicate	
14986	67 Citric acid	[945; Galactofuranose-6-phosphate (7TMS)]	123	-0,004	-0,138	15,201	0,466	69	73	77	65	43	22 original
7223	67 Citric acid	[548; Leucine (2TBS)]	60	-0,021	-0,035	19,350	0,389	70	72	77	65	65	103 duplicate
7203	67 Citric acid	[644; Erythritol (4TMS)]	122	-0,023	-0,097	31,227	0,425	71	71	72	70	121	66 original
10423	67 Citric acid	[904; Galactose methoxyamine (5TMS)]	64	-0,032	-0,048	24,676	0,344	72	70	69	73	92	133 original
12236	67 Citric acid	Phosphoric acid	51	-0,032	0,362	12,155	0,413	73	69	48	98	24	73 duplicate
7185	67 Citric acid	[590; 1-Acetyl-2-thiohydantoin]	64	-0,044	-0,052	18,779	0,348	74	68	70	72	59	132 duplicate
7228	67 Citric acid	Mannitol	62	-0,045	-0,567	14,663	0,489	75	67	116	26	41	21 original
7201	67 Citric acid	[777; Fructose-6-phosphate methoxyamine (6TMS)]	39	-0,050	-0,163	16,882	0,272	76	66	78	64	51	140 original
7194	67 Citric acid	[857; Mannitol (6TMS)]	100	-0,056	-0,162	17,318	0,334	77	65	80	82	52	137 original
7197	67 Citric acid	[607; Putrescine (4TMS)]	64	-0,058	-0,358	34,787	0,454	78	64	84	84	129	43 original
7233	67 Citric acid	myo-Inositol	49	-0,070	-0,038	38,781	0,410	79	63	68	74	135	79 original
7205	67 Citric acid	[895; Isomaltose methoxyamine (8TMS)]	132	-0,080	-0,390	29,081	0,327	80	62	98	44	115	138 original
7211	67 Citric acid	[795; Erythritol (4TMS)]	104	-0,081	-0,118	22,245	0,449	81	61	74	68	80	51 original
7213	67 Citric acid	[715; Erythritol (4TMS)]	54	-0,082	-0,211	26,355	0,450	82	60	82	60	103	50 original
7222	67 Citric acid	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	110	-0,086	-0,125	36,033	0,413	83	59	75	67	134	74 original
7229	67 Citric acid	[657; Erythritol (4TMS)]	121	-0,110	-0,099	31,118	0,352	84	58	73	69	120	129 original
7173	67 Citric acid	[824; D-Scotoheptulose-7-phosphate (7TMS)]	128	-0,111	-0,227	16,008	0,304	85	57	84	58	46	139 original
15911	67 Citric acid	[919; D-Xylopyranose (4TMS)]	72	-0,124	-0,155	25,938	0,353	86	56	79	63	99	128 original
14789	67 Citric acid	Glycerol-2-phosphate	53	-0,127	-0,220	29,940	0,342	87	55	83	59	117	135 duplicate
7218	67 Citric acid	[639; Proline (2TMS)]	41	-0,146	-0,134	12,715	0,461	88	54	76	68	30	35 duplicate
12358	67 Citric acid	[724; Glycerol (3TMS)]	117	-0,151	-0,193	23,495	0,402	89	53	81	61	87	88 original
7216	67 Citric acid	Alanine (BP) (3TMS)	19	-0,161	-0,277	15,751	0,517	90	52	86	56	45	14 duplicate
7180	67 Citric acid	Glucose-6-phosphate	62	-0,169	-0,468	8,462	0,416	91	51	105	37	7	71 original
7219	67 Citric acid	Glucose	64	-0,173	-0,423	14,222	0,483	92	50	101	41	35	23 original
14174	67 Citric acid	[928; Glucopyranose-6-phosphate (6TMS)]	35	-0,175	-0,323	25,004	0,349	93	49	92	50	95	131 original
11864	67 Citric acid	Pyroglutamic acid	64	-0,176	-0,488	18,652	0,461	94	48	107	35	60	34 duplicate
13411	67 Citric acid	Alanine	15	-0,197	-0,321	10,535	0,440	95	47	91	51	13	57 duplicate
7174	67 Citric acid	Malic acid	64	-0,219	-0,401	16,702	0,404	96	46	99	43	50	85 duplicate
14689	67 Citric acid	[708; Glucose methoxyamine (5TMS)]	73	-0,224	-0,294	26,266	0,403	97	45	88	54	102	87 original
12599	67 Citric acid	[680; 2,3-Olimethylsuccinic acid (2TMS)]	40	-0,225	-0,300	11,478	0,384	98	44	89	53	19	104 duplicate
13184	67 Citric acid	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	21	-0,234	-0,344	9,514	0,349	99	43	89	49	11	130 duplicate
7221	67 Citric acid	Citramalic acid	64	-0,239	-0,314	8,465	0,409	100	42	90	52	8	80 duplicate
12178	67 Citric acid	[945; Uridine (3TMS)]	120	-0,241	-0,270	12,591	0,362	102	40	85	57	27	122 original
7177	67 Citric acid	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	22	-0,244	-0,428	29,292	0,342	103	39	102	40	116	134 duplicate
11483	67 Citric acid	Fructose	64	-0,251	-0,540	12,910	0,457	104	38	111	31	32	39 original
7179	67 Citric acid	Glyceral acid	63	-0,251	-0,432	30,123	0,338	105	37	103	39	118	136 duplicate
		Mannose	62	-0,273	-0,443	27,838	0,399	106	36	104	38	108	83 original



7226	67 Citric acid	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	-0.280	-0.609	14.391	0.438	107	35	121	21	37	59 original
7207	67 Citric acid	106	[733; Threitol (4TMS)]	62	-0.293	-0.403	17.228	0.541	108	34	100	42	74	7 original
7206	67 Citric acid	105	[705; 2-Ketogluconic acid (5TMS)]	48	-0.298	-0.489	17.949	0.365	109	33	108	34	56	118 original
11738	67 Citric acid	14	Fumaric acid	64	-0.313	-0.469	28.111	0.397	110	32	106	38	10	97 duplicate
7193	67 Citric acid	92	[680; Glycerol-2-phosphate (4TMS)]	54	-0.340	-0.574	22.281	0.356	111	31	117	25	81	127 original
7171	67 Citric acid	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	-0.346	-0.389	9.935	0.402	112	30	97	45	12	89 original
14486	67 Citric acid	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.363	-0.527	19.557	0.410	113	29	110	32	66	77 duplicate
11354	67 Citric acid	11	Succinic acid	64	-0.372	-0.511	18.864	0.364	114	28	109	33	61	119 duplicate
16731	67 Citric acid	62	[812; D-Xylofuranose (4TMS)]	64	-0.377	-0.545	11.723	0.431	115	28	112	30	22	62 duplicate
10694	67 Citric acid	6	Glycerol	64	-0.377	-0.600	19.190	0.468	116	27	119	23	63	29 duplicate
15998	67 Citric acid	54	[NA]	55	-0.378	-0.562	28.516	0.394	117	25	115	27	112	99 duplicate
13523	67 Citric acid	29	Erythritol	64	-0.379	-0.553	22.735	0.403	118	24	113	29	83	88 duplicate
16326	67 Citric acid	57	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55	-0.430	-0.607	21.398	0.370	119	23	120	22	77	115 duplicate
7187	67 Citric acid	86	[793; D-Galactono-1,4-lactone (4TMS)]	61	-0.435	-0.679	22.829	0.489	120	22	134	8	86	20 original
14588	67 Citric acid	39	[829; 1-Phenylethanol (1TMS)]	63	-0.439	-0.578	18.748	0.361	121	21	118	24	58	123 duplicate
7189	67 Citric acid	88	Gluconic acid	64	-0.464	-0.670	19.198	0.465	122	20	129	13	64	31 original
7200	67 Citric acid	99	[682; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	-0.468	-0.557	24.398	0.371	123	19	114	28	91	114 original
15368	67 Citric acid	47	[NA]	64	-0.470	-0.610	23.832	0.435	124	18	122	20	88	61 duplicate
7198	67 Citric acid	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	-0.472	-0.739	17.612	0.440	125	17	140	2	54	55 original
12953	67 Citric acid	24	[755; 2-Ketooctanoic acid (2TMS)]	64	-0.481	-0.654	12.395	0.459	126	16	128	14	28	37 duplicate
7230	67 Citric acid	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	-0.483	-0.636	24.691	0.410	127	15	123	19	93	78 original
12113	67 Citric acid	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	-0.490	-0.639	12.204	0.405	128	14	124	18	25	84 duplicate
16242	67 Citric acid	56	[829; Orolic acid (3TMS)]	64	-0.492	-0.674	28.106	0.460	129	13	132	10	109	36 duplicate
11989	67 Citric acid	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	-0.495	-0.645	10.678	0.452	130	12	127	15	16	45 duplicate
7204	67 Citric acid	103	[648; Ethylamine (2TMS)]	63	-0.504	-0.687	22.804	0.392	131	11	135	7	85	100 original
16962	67 Citric acid	65	[646; 3-Deoxyglucitol (5TMS)]	63	-0.509	-0.639	28.901	0.476	132	10	125	17	113	28 duplicate
15644	67 Citric acid	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	-0.510	-0.640	37.862	0.391	133	9	126	16	137	101 duplicate
7235	67 Citric acid	134	Isomaltose	64	-0.515	-0.672	18.158	0.452	134	8	131	11	47	47 original
15274	67 Citric acid	46	Arabinose	64	-0.518	-0.689	21.456	0.450	135	7	136	6	78	49 duplicate
10009	67 Citric acid	1	[938; Sulfuric acid (2TMS)]	36	-0.540	-0.718	18.993	0.375	136	6	138	4	62	110 duplicate
7181	67 Citric acid	80	[772; D-Glucose (5TMS)]	62	-0.541	-0.670	14.560	0.409	137	6	130	12	39	81 original
7202	67 Citric acid	101	[832; Dopamine (4TMS)]	64	-0.549	-0.733	22.623	0.430	138	3	139	3	82	64 original
7192	67 Citric acid	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	-0.549	-0.771	25.949	0.419	139	4	141	1	100	69 original
11611	67 Citric acid	13	Uracil	64	-0.572	-0.678	14.323	0.452	140	2	133	9	36	48 duplicate
7188	67 Citric acid	87	[945; beta-D-Glucopyranose (5TMS)]	62	-0.616	-0.703	17.415	0.455	141	1	137	5	63	41 original
15462	68 [570; Hypoxanthine (2T)]	48	Asparagine	20	0.842	0.958	17.879	0.639	1	139	3	137	86	2 duplicate
15824	68 [570; Hypoxanthine (2T)]	52	[NA]	19	0.825	0.943	8.763	0.581	2	138	10	130	17	28 duplicate
15735	68 [570; Hypoxanthine (2T)]	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	16	0.817	0.876	2.751	0.570	3	137	20	120	1	31 duplicate
10962	68 [570; Hypoxanthine (2T)]	8	Isolaudine	18	0.752	0.539	19.998	0.434	4	136	40	100	100	79 duplicate
11225	68 [570; Hypoxanthine (2T)]	10	Glycine	20	0.747	0.949	23.590	0.616	5	135	8	132	116	11 duplicate
16085	68 [570; Hypoxanthine (2T)]	55	[612; 4-Aminobutyric acid (2TBS)]	14	0.736	0.989	3.538	0.609	6	134	1	139	2	16 duplicate
14384	68 [570; Hypoxanthine (2T)]	37	Phenylalanine	20	0.716	0.811	24.797	0.545	7	132	24	116	118	43 duplicate
13635	68 [570; Hypoxanthine (2T)]	30	[815; Ethyl-3(2H)-thiophenone]	20	0.716	0.702	28.590	0.429	8	133	31	109	129	83 duplicate
10287	68 [570; Hypoxanthine (2T)]	3	Ethanolamine	19	0.708	0.939	11.164	0.624	9	131	11	129	35	6 duplicate
12837	68 [570; Hypoxanthine (2T)]	23	Homoserine	20	0.705	0.953	15.162	0.567	10	129	7	133	67	34 duplicate
13745	68 [570; Hypoxanthine (2T)]	31	[622; Parabanic acid (2TMS)]	20	0.705	0.734	10.214	0.476	11	130	27	113	26	62 duplicate
16810	68 [570; Hypoxanthine (2T)]	63	Glutamine	20	0.695	0.954	16.684	0.553	12	128	5	135	81	41 duplicate
7255	68 [570; Hypoxanthine (2T)]	81	Tyrosine	20	0.684	0.888	33.267	0.571	13	126	17	123	135	29 original
16653	68 [570; Hypoxanthine (2T)]	61	[NA]	20	0.684	0.825	14.258	0.442	14	127	23	117	59	77 duplicate

13962	68 [570]: Hypoxanthine (2T)	33	Methionine	20	0.653	0.715	15,066	0.528	15	124	29	111	65	51 duplicate
11094	68 [570]: Hypoxanthine (2T)	9	Proline	20	0.653	0.667	26,103	0.430	16	125	34	106	121	82 duplicate
10149	68 [570]: Hypoxanthine (2T)	2	Serine	19	0.649	0.682	19,453	0.499	17	123	33	107	96	56 duplicate
15180	68 [570]: Hypoxanthine (2T)	45	Homocysteine	19	0.637	0.714	4,088	0.476	18	122	30	110	4	63 duplicate
10560	68 [570]: Hypoxanthine (2T)	5	Leucine	16	0.633	0.859	9,078	0.557	19	121	22	118	20	38 duplicate
7251	68 [570]: Hypoxanthine (2T)	77	[826; beta-[[[5-methyl-2-thienyl)methyl]amino- benzeneacetic acid methyl ester]	18	0.621	0.903	28,689	0.594	20	120	16	124	131	20 original
7272	68 [570]: Hypoxanthine (2T)	98	[897; Ribose-5-phosphate methoxyamine (5TMS)]	16	0.583	0.881	3,540	0.531	21	119	19	121	3	48 original
7263	68 [570]: Hypoxanthine (2T)	89	[775; Dopamine (4TMS)]	15	0.581	0.983	12,342	0.586	22	118	2	138	46	25 original
16573	68 [570]: Hypoxanthine (2T)	60	Glycerol-3-phosphate	20	0.568	0.889	24,536	0.533	23	117	32	108	117	47 duplicate
14889	68 [570]: Hypoxanthine (2T)	42	Glutamic acid	19	0.567	0.864	28,072	0.547	24	116	21	119	127	42 duplicate
7305	68 [570]: Hypoxanthine (2T)	131	[626; 5-Methylthioadenosine (3TMS)]	15	0.562	0.931	5,462	0.554	25	115	13	127	10	40 original
13070	68 [570]: Hypoxanthine (2T)	25	[709; 2,5-Diaminovalerolactam (2TMS)]	10	0.556	0.924	8,707	0.213	26	114	14	126	16	132 duplicate
17112	68 [570]: Hypoxanthine (2T)	67	Citric acid	20	0.547	0.757	25,532	0.541	27	113	25	115	119	45 duplicate
7269	68 [570]: Hypoxanthine (2T)	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	17	0.544	0.911	4,334	0.636	28	112	15	125	6	3 original
13854	68 [570]: Hypoxanthine (2T)	32	[729; N,N-Dimethyllysine methyl ester]	19	0.544	0.887	10,690	0.587	29	111	18	122	31	24 duplicate
14069	68 [570]: Hypoxanthine (2T)	34	Aspartic acid	20	0.526	0.717	30,539	0.505	30	110	28	112	133	55 duplicate
10829	68 [570]: Hypoxanthine (2T)	7	Threonine	20	0.474	0.578	28,639	0.426	31	109	39	101	130	86 duplicate
7243	68 [570]: Hypoxanthine (2T)	69	Arginine	19	0.462	0.932	23,558	0.612	32	108	12	128	115	13 original
17038	68 [570]: Hypoxanthine (2T)	66	Glycine acid-3-phosphate	20	0.453	0.586	12,302	0.462	33	107	37	103	45	69 duplicate
13299	68 [570]: Hypoxanthine (2T)	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	18	0.412	0.954	6,702	0.288	34	106	6	134	14	33 duplicate
7282	68 [570]: Hypoxanthine (2T)	108	Oxalacetic acid	20	0.400	0.485	12,841	0.288	35	105	42	98	50	122 original
14987	68 [570]: Hypoxanthine (2T)	43	[548; Leucine (2TBS)]	19	0.392	0.636	13,828	0.568	36	104	35	105	57	35 duplicate
16492	68 [570]: Hypoxanthine (2T)	59	Omitline; Arginine	20	0.368	0.745	35,163	0.544	37	103	26	114	139	44 duplicate
7302	68 [570]: Hypoxanthine (2T)	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	7	0.333	0.315	15,041	0.165	38	101	48	92	64	133 original
7279	68 [570]: Hypoxanthine (2T)	105	[705; 2-Ketoglucuronic acid (5TMS)]	7	0.333	0.201	15,382	0.084	39	102	51	89	71	135 original
15554	68 [570]: Hypoxanthine (2T)	49	[877; Pyrophosphoric acid (4TMS)]	20	0.295	0.533	10,263	0.408	40	100	41	99	27	93 duplicate
7245	68 [570]: Hypoxanthine (2T)	71	[731; Erythrose (3TMS)]	20	0.284	0.333	18,403	0.419	41	99	46	94	89	90 original
7249	68 [570]: Hypoxanthine (2T)	75	Lysine	20	0.263	0.454	33,323	0.369	42	98	43	97	137	105 original
7256	68 [570]: Hypoxanthine (2T)	82	Lysine	16	0.250	0.945	20,885	0.636	43	97	9	131	105	4 original
7293	68 [570]: Hypoxanthine (2T)	119	[931; myo-Inositol-2-phosphate (7TMS)]	20	0.242	0.630	16,372	0.478	44	96	36	104	79	60 original
7281	68 [570]: Hypoxanthine (2T)	107	9-(Z)-Octadecenoic acid	20	0.211	0.413	20,563	0.365	45	95	44	96	101	107 original
7311	68 [570]: Hypoxanthine (2T)	137	Ergosterol	20	0.168	0.282	19,968	0.368	46	94	49	91	99	106 original
10424	68 [570]: Hypoxanthine (2T)	4	Phosphoric acid	15	0.162	0.395	26,788	0.349	47	93	45	95	122	111 duplicate
7267	68 [570]: Hypoxanthine (2T)	93	[607; Pureschne (4TMS)]	19	0.158	-0.116	9,284	0.451	48	92	58	82	21	74 original
14280	68 [570]: Hypoxanthine (2T)	36	[596; N-Acetylglutamic acid (2TMS)]	20	0.147	0.586	27,578	0.361	49	91	38	102	123	109 duplicate
7257	68 [570]: Hypoxanthine (2T)	83	Sorbitol	18	0.124	0.126	21,432	0.393	50	90	54	86	107	98 original
12480	68 [570]: Hypoxanthine (2T)													
7315	68 [570]: Hypoxanthine (2T)	141	[619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	14	0.077	0.957	5,332	0.615	51	89	4	136	9	12 duplicate
7285	68 [570]: Hypoxanthine (2T)	111	Lanosta-8,24-dien-3-beta-ol	20	0.032	0.159	9,293	0.420	52	88	53	87	22	88 original
7264	68 [570]: Hypoxanthine (2T)	141	[583; Erythritol (4TMS)]	10	0.022	-0.084	4,191	0.018	53	87	57	83	5	137 original
7313	68 [570]: Hypoxanthine (2T)	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	20	0.011	0.055	15,877	0.429	54	86	55	85	74	84 original
7270	68 [570]: Hypoxanthine (2T)	139	[700; Ergosta-5,7-dien-3-ol]	15	0.010	0.264	4,598	0.247	55	85	50	90	7	128 original
7200	68 [570]: Hypoxanthine (2T)	96	myo-Inositol	19	0.006	0.478	5,890	0.334	56	84	72	68	11	115 original
7268	68 [570]: Hypoxanthine (2T)	126	[559; Erythritol (4TMS)]	7	-0.048	-0.204	11,627	0.083	57	83	64	76	39	136 original
	68 [570]: Hypoxanthine (2T)	94	Hexadecanoic acid	20	-0.074	-0.461	23,448	0.433	58	82	71	69	113	80 original
7298	68 [570]: Hypoxanthine (2T)	124	[734; 1-Monooleoylglycerol (2TMS); 1-Monoheptadecanoylglycerol (1TMS)]											
7246	68 [570]: Hypoxanthine (2T)	72	[919; D-Xylopyranose (4TMS)]	19	-0.076	0.185	4,810	0.389	59	81	52	88	8	100 original
7283	68 [570]: Hypoxanthine (2T)	109	Oxalacetic acid	19	-0.099	-0.020	12,283	0.312	60	80	56	84	44	119 original
	68 [570]: Hypoxanthine (2T)			20	-0.105	-0.546	22,683	0.401	61	79	76	64	109	95 original

16410	68 [570]: Hypoxanthine (2T)	58 [1TMS]	636: 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane	20 -0.116	0.321	19.334	0.403	62	78	47	93	95	94 duplicate
10010	68 [570]: Hypoxanthine (2T)	1 [938]: Sulfuric acid (2TMS)		8 -0.143	-0.514	11.899	-0.047	63	77	74	68	41	139 duplicate
7247	68 [570]: Hypoxanthine (2T)	73 [708]: Glucose methoxymine (5TMS)		17 -0.147	-0.865	11.064	0.530	64	76	102	38	34	49 original
7290	68 [570]: Hypoxanthine (2T)	116 [882]: Pseudouridine (5TMS)		12 -0.152	-0.424	9.017	0.284	65	75	69	71	19	124 original
7309	68 [570]: Hypoxanthine (2T)	135											
16887	68 [570]: Hypoxanthine (2T)	64 [789]: Tyramine (3TMS)	[902: Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	20 -0.179	-0.651	18.439	0.399	66	74	78	62	90	96 original
7312	68 [570]: Hypoxanthine (2T)	138 [674]: Ergosterol (1TMS)		19 -0.181	-0.432	12.175	0.290	67	73	70	70	42	121 duplicate
7314	68 [570]: Hypoxanthine (2T)	140 [692]: Ergosta-7,22-dien-3-ol (1TMS)		18 -0.203	-0.196	6.259	0.331	68	72	63	77	12	117 original
14487	68 [570]: Hypoxanthine (2T)	38 [708]: 2,3-Dimethylsuccinic acid (2TMS)		19 -0.205	-0.178	6.419	0.388	69	71	61	79	13	101 original
7304	68 [570]: Hypoxanthine (2T)	130 Trehalose		19 -0.211	-0.892	15.174	0.506	70	70	111	29	68	54 duplicate
13524	68 [570]: Hypoxanthine (2T)	29 Erythritol		19 -0.216	-0.185	27.791	0.340	71	69	62	78	125	114 original
11990	68 [570]: Hypoxanthine (2T)	16 [644]: 2-Methyl-1,3-butanediol (2TMS)		20 -0.221	-0.883	13.382	0.509	72	67	107	33	54	53 duplicate
7301	68 [570]: Hypoxanthine (2T)	127 [777]: Fructose-6-phosphate methoxymine (8TMS)		20 -0.221	-0.804	21.031	0.633	73	68	118	22	106	5 duplicate
7286	68 [570]: Hypoxanthine (2T)	112 [877]: beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)		7 -0.238	-0.157	12.561	0.002	74	68	60	80	48	138 original
14589	68 [570]: Hypoxanthine (2T)	39 [829]: 1-Phenylethanol (1TMS)		20 -0.242	-0.681	7.227	0.473	75	64	80	60	15	65 original
7307	68 [570]: Hypoxanthine (2T)	133 [835]: Squalene		20 -0.242	-0.808	19.293	0.583	76	65	122	18	94	26 duplicate
11484	68 [570]: Hypoxanthine (2T)	12 Glyceric acid		20 -0.253	-0.240	14.320	0.318	77	63	65	75	60	118 original
12954	68 [570]: Hypoxanthine (2T)	24 [725]: 2-Keitoctanoic acid (2TMS)		19 -0.263	-0.835	10.288	0.419	78	61	95	45	28	89 duplicate
12114	68 [570]: Hypoxanthine (2T)	17 [700]: 2-methyl-1,2-propanediol (2TMS)		20 -0.263	-0.914	28.487	0.619	79	62	124	16	128	9 duplicate
16963	68 [570]: Hypoxanthine (2T)	85 [646]: 3-Deoxyglucitol (5TMS)		20 -0.274	-0.892	20.605	0.570	80	59	110	30	102	30 duplicate
7294	68 [570]: Hypoxanthine (2T)	120 [945]: Uridine (3TMS)		15 -0.276	-0.916	15.338	0.619	81	60	125	15	70	8 duplicate
11885	68 [570]: Hypoxanthine (2T)	15 Alanine		20 -0.284	-0.300	16.777	0.397	82	58	66	74	83	97 original
7258	68 [570]: Hypoxanthine (2T)	84 Mannitol		19 -0.287	-0.387	29.370	0.457	83	57	105	35	93	39 duplicate
7274	68 [570]: Hypoxanthine (2T)	100 [857]: Mannitol (6TMS)		20 -0.295	-0.673	16.357	0.458	84	56	67	73	132	72 original
16243	68 [570]: Hypoxanthine (2T)	56 [829]: Citric acid (3TMS)		20 -0.305	-0.926	13.986	0.621	85	54	79	61	78	71 original
7277	68 [570]: Hypoxanthine (2T)	103 [648]: Ethylamine (2TMS)		20 -0.305	-0.774	16.100	0.598	86	55	133	7	58	7 duplicate
10695	68 [570]: Hypoxanthine (2T)	6 Glycerol		20 -0.305	-0.831	33.577	0.371	88	53	94	46	138	104 duplicate
7276	68 [570]: Hypoxanthine (2T)	102 [804]: Galactose methoxymine (5TMS)		20 -0.316	-0.524	12.446	0.452	89	51	75	65	47	73 original
15084	68 [570]: Hypoxanthine (2T)	44 [910]: 2-Ketogluconic acid methoxymine (4TMS)		9 -0.333	-0.765	14.517	0.113	90	48	87	53	62	134 duplicate
7273	68 [570]: Hypoxanthine (2T)	99 [662]: Ribose-5-phosphate methoxymine (BP) (5TMS)		12 -0.333	-0.845	11.274	0.229	91	49	98	42	36	130 original
7287	68 [570]: Hypoxanthine (2T)	113 Galactose-6-phosphate		19 -0.333	-0.862	11.679	0.412	92	50	101	39	40	91 original
7303	68 [570]: Hypoxanthine (2T)	129 [840]: Maltose methoxymine (8TMS); alpha-D-Glc-(1,4)-D-Glc		17 -0.338	-0.900	15.144	0.489	93	47	115	25	66	57 original
15912	68 [570]: Hypoxanthine (2T)	53 Glycerol-2-phosphate		20 -0.347	-0.157	10.036	0.344	94	43	59	81	25	113 duplicate
12237	68 [570]: Hypoxanthine (2T)	18 [590]: 1-Acetyl-2-thiohydantoin		20 -0.347	-0.631	15.463	0.411	95	44	77	63	72	92 duplicate
7265	68 [570]: Hypoxanthine (2T)	91 [766]: beta-D-Methylglucopyranoside (4TMS)		20 -0.347	-0.685	16.777	0.568	96	45	81	59	82	32 original
11355	68 [570]: Hypoxanthine (2T)	11 Succinic acid		20 -0.347	-0.868	15.259	0.470	97	46	103	37	69	66 duplicate
15275	68 [570]: Hypoxanthine (2T)	46 Arabinose		20 -0.358	-0.921	19.065	0.617	98	42	130	10	92	10 duplicate
7271	68 [570]: Hypoxanthine (2T)	97 [756]: beta-D-Methylglucopyranoside (4TMS)		11 -0.382	-0.820	19.689	0.251	99	41	90	50	88	127 original
7244	68 [570]: Hypoxanthine (2T)	70 [693]: 2-Furan-2-hydroxyacetic acid (2TMS)		18 -0.388	-0.830	18.179	0.359	100	40	92	48	88	110 original
7289	68 [570]: Hypoxanthine (2T)	115 Glucose-6-phosphate		19 -0.392	-0.905	23.391	0.466	101	39	119	21	112	67 original
14175	68 [570]: Hypoxanthine (2T)	35 Pyroglutamic acid		20 -0.400	-0.929	33.310	0.468	102	38	136	4	136	14 duplicate
15369	68 [570]: Hypoxanthine (2T)	47 [NA]		20 -0.411	-0.396	14.870	0.240	103	33	68	72	63	128 duplicate
7278	68 [570]: Hypoxanthine (2T)	104 [795]: Erythritol (4TMS)		20 -0.411	-0.708	13.454	0.528	104	34	84	56	56	52 original
7250	68 [570]: Hypoxanthine (2T)	76 Fructose		20 -0.411	-0.919	23.023	0.583	105	35	129	11	110	27 original
7299	68 [570]: Hypoxanthine (2T)	125 [892]: Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru		20 -0.411	-0.922	25.897	0.535	106	36	131	9	120	46 original
7308	68 [570]: Hypoxanthine (2T)	134 Isomaltose		20 -0.411	-0.928	23.356	0.592	107	37	135	5	111	21 original
13185	68 [570]: Hypoxanthine (2T)	26 Citramalic acid		20 -0.421	-0.842	20.643	0.430	108	31	97	43	103	81 duplicate
7262	68 [570]: Hypoxanthine (2T)	88 Gluconic acid		20 -0.421	-0.917	17.203	0.644	109	32	126	14	85	1 original

7275	68 [570]: Hypoxanthine (2T) 101 [832]: Dopamine (4TMS)]	20 -0.432	-0.893	14.385	0.564	110	27	82	58	61	36 original	
7253	68 [570]: Hypoxanthine (2T) 79 Glucose	20 -0.432	-0.823	27.678	0.442	111	28	91	49	124	76 original	
11612	68 [570]: Hypoxanthine (2T) 13 Uracil	20 -0.432	-0.924	19.616	0.610	112	29	132	8	97	15 duplicate	
7260	68 [570]: Hypoxanthine (2T) 86 [793]: D-Galactono-1,4-lactone (4TMS)]	20 -0.432	-0.927	21.469	0.603	113	30	134	6	108	18 original	
7282	68 [570]: Hypoxanthine (2T) 118 [928]: Glucopyranose-6-phosphate (6TMS)]	17 -0.441	-0.509	10.641	0.271	114	26	73	67	30	125 original	
12600	68 [570]: Hypoxanthine (2T) 21 [678]: N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	20 -0.442	-0.791	20.812	0.421	115	24	89	51	104	87 duplicate	
13412	68 [570]: Hypoxanthine (2T) 28 Malic acid	20 -0.442	-0.941	16.300	0.588	116	25	138	2	77	23 duplicate	
7248	68 [570]: Hypoxanthine (2T) 74 [912]: Tetradecanoic acid (1TMS)]	20 -0.453	-0.730	13.311	0.464	117	23	85	55	53	68 original	
15989	68 [570]: Hypoxanthine (2T) 54 [NA]	12 -0.455	-0.893	12.222	0.333	118	22	112	28	43	116 duplicate	
16327	57 [757]: 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	14 -0.473	-0.917	17.186	0.309	119	21	127	13	84	120 duplicate	
7252	68 [570]: Hypoxanthine (2T) 78 Mannose	20 -0.474	-0.831	12.807	0.460	120	19	93	47	49	70 original	
7297	68 [570]: Hypoxanthine (2T) 123 [945]: Galactofuranose-6-phosphate (7TMS)]	20 -0.474	-0.873	16.131	0.590	121	20	104	36	76	22 original	
7288	68 [570]: Hypoxanthine (2T) 114 Fructose-6-phosphate	18 -0.477	-0.837	10.922	0.392	122	18	96	44	32	99 original	
14690	68 [570]: Hypoxanthine (2T) 40 [680]: 2,3-Dimethylsuccinic acid (2TMS)]	20 -0.484	-0.858	30.818	0.558	123	17	100	40	134	37 duplicate	
14790	68 [570]: Hypoxanthine (2T) 41 [639]: Proline (2TMS)]	20 -0.495	-0.704	18.081	0.438	124	16	83	57	87	78 duplicate	
7280	68 [570]: Hypoxanthine (2T) 106 [733]: Threitol (4TMS)]	20 -0.516	-0.900	15.773	0.605	125	15	116	24	73	17 original	
12719	68 [570]: Hypoxanthine (2T) 22 [690]: N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	15 -0.524	-0.949	9.673	0.387	126	14	139	1	23	102 duplicate	
7259	68 [570]: Hypoxanthine (2T) 85 [528]: Methylcitric acid (4TMS)]	16 -0.533	-0.753	10.605	0.426	127	13	86	54	29	85 original	
16732	68 [570]: Hypoxanthine (2T) 62 [812]: D-Xylofuranose (4TMS)]	20 -0.537	-0.884	18.743	0.474	128	11	108	32	91	64 duplicate	
11738	68 [570]: Hypoxanthine (2T) 14 Fumaric acid	20 -0.537	-0.932	10.958	0.529	129	12	137	3	33	50 duplicate	
15645	68 [570]: Hypoxanthine (2T) 50 [746]: Ribonic acid-1,4-lactone (3TMS)]	11 -0.564	-0.919	12.952	0.483	130	10	117	23	18	59 duplicate	
7266	68 [570]: Hypoxanthine (2T) 92 [690]: Glyceral-2-phosphate (4TMS)]	16 -0.583	-0.895	13.100	0.451	132	8	114	26	52	131 original	
7291	68 [570]: Hypoxanthine (2T) 117 [724]: Glycerol (3TMS)]	11 -0.600	-0.908	11.550	0.288	133	7	121	19	38	123 original	
7284	68 [570]: Hypoxanthine (2T) 122 [644]: Erythritol (4TMS)]	13 -0.641	-0.913	13.426	0.383	134	6	123	17	55	103 original	
12359	68 [570]: Hypoxanthine (2T) 110 [715]: Erythritol (4TMS)]	20 -0.674	-0.880	16.375	0.484	135	5	106	34	80	58 duplicate	
7306	68 [570]: Hypoxanthine (2T) 132 [895]: Isomaltose methoxyamine (8TMS)]	10 -0.689	-0.908	11.428	0.262	136	4	120	20	37	128 original	
7261	68 [570]: Hypoxanthine (2T) 87 [945]: beta-D-Glucopyranose (5TMS)]	20 -0.695	-0.893	27.827	0.363	137	3	113	27	126	108 original	
7254	68 [570]: Hypoxanthine (2T) 80 [772]: D-Glucose (5TMS)]	19 -0.719	-0.855	23.460	0.347	138	2	99	41	114	112 original	
7295	68 [570]: Hypoxanthine (2T) 121 [657]: Erythritol (4TMS)]	15 -0.733	-0.888	9.980	0.478	139	1	109	31	24	61 original	
7310	68 [570]: Hypoxanthine (2T) 136 [748]: D-Sedoheptulose-7-phosphate (7TMS)]	0				140	140	140	140	140	140 original	
16493	69 Arginine	60 0.771	0.937	23.872	0.620	1	141	1	141	92	20 duplicate	
13638	69 Arginine	60 0.763	0.895	12.244	0.552	2	140	7	135	15	58 duplicate	
7328	69 Arginine	39 0.762	0.923	7.750	0.655	3	139	4	138	3	4 original	
14890	69 Arginine	59 0.753	0.911	10.176	0.593	4	138	5	137	6	41 duplicate	
7327	69 Arginine	60 0.747	0.868	15.615	0.594	5	137	13	129	34	38 original	
7323	69 Arginine	59 0.746	0.891	10.913	0.597	6	136	10	132	10	35 original	
13963	69 Arginine	60 0.725	0.858	14.279	0.577	7	135	14	128	23	44 duplicate	
13855	69 Arginine	60 0.678	0.834	22.037	0.688	8	133	2	140	75	1 duplicate	
11226	69 Arginine	60 0.678	0.896	5.682	0.620	9	134	6	136	2	21 duplicate	
15736	69 Arginine	51 [499]: 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	43 0.674	0.883	33.680	0.594	10	132	12	130	136	39 duplicate
10561	69 Arginine	5 Leucine	45 0.636	0.891	21.453	0.637	11	131	11	131	69	12 duplicate
14070	69 Arginine	34 Aspartic acid	60 0.634	0.795	16.154	0.566	12	130	17	125	38	53 duplicate
15463	69 Arginine	48 Asparagine	60 0.619	0.822	15.481	0.614	13	129	16	126	31	26 duplicate
10288	69 Arginine	3 Ethanolamine	59 0.619	0.773	23.419	0.535	14	128	19	123	89	66 duplicate
14385	69 Arginine	37 Phenylalanine	60 0.598	0.764	10.304	0.542	15	127	20	122	8	62 duplicate
11095	69 Arginine	9 Proline	59 0.596	0.727	11.015	0.549	16	126	23	119	11	61 duplicate
10963	69 Arginine	8 Isoleucine	55 0.589	0.634	11.038	0.433	17	125	31	111	12	124 duplicate
16086	69 Arginine	55 [612]: 4-Aminobutyric acid (2TBS)]	43 0.588	0.668	36.651	0.529	18	124	28	114	139	68 duplicate

15181	69 Arginine	45 Homocysteine	57 0.559	0.679	35.513	0.513	19	123	27	115	138	85 duplicate
13746	69 Arginine	31 [622; Parabenic acid (2TMS)]	60 0.558	0.775	23.874	0.550	20	122	18	124	93	60 duplicate
15555	69 Arginine	49 [877; Pyrophosphoric acid (4TMS)]	60 0.537	0.623	32.002	0.499	21	121	33	109	132	92 duplicate
13071	69 Arginine	25 [709; 2,5-Diaminovaleic acid (2TMS)]	44 0.522	0.891	16.631	0.616	22	120	9	133	40	25 duplicate
13300	69 Arginine	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	52 0.516	0.892	27.936	0.618	23	119	8	134	115	23 duplicate
7341	69 Arginine	95 [770; 3,4,6-Trisubstitutedphenylthioaniline (5TMS)]	47 0.515	0.595	33.489	0.495	24	118	35	107	135	93 original
7377	69 Arginine	131 [826; 5-Methylthioadenosine (3TMS)]	51 0.507	0.573	30.017	0.562	25	117	38	104	128	55 original
17113	69 Arginine	67 Citric acid	60 0.495	0.631	11.518	0.492	26	116	32	110	13	98 duplicate
7355	69 Arginine	89 [775; Dopamine (4TMS)]	35 0.492	0.717	23.271	0.571	27	115	24	118	84	49 original
10150	69 Arginine	2 Serine	60 0.489	0.695	9.927	0.515	28	114	26	116	5	82 duplicate
7382	69 Arginine	138 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17 0.485	0.712	4.519	0.488	29	113	25	117	1	101 original
12838	69 Arginine	23 Homoserine	60 0.482	0.855	14.536	0.655	30	112	15	127	25	2 duplicate
16574	69 Arginine	60 Glycerol-3-phosphate	60 0.478	0.597	9.913	0.516	31	111	34	108	4	79 duplicate
17186	69 Arginine	68 [570; Hypoxanthine (2TMS)]	19 0.462	0.932	23.558	0.612	32	110	3	139	90	28 duplicate
17039	69 Arginine	66 Glycine acid-3-phosphate	60 0.429	0.659	20.565	0.516	33	109	29	113	64	81 duplicate
16654	69 Arginine	61 [NA]	60 0.428	0.420	18.579	0.468	34	108	43	99	48	111 duplicate
10830	69 Arginine	7 Threonine	60 0.424	0.656	15.312	0.519	35	107	30	112	28	72 duplicate
7344	69 Arginine	98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	45 0.406	0.748	30.114	0.639	36	106	21	121	129	11 original
15825	69 Arginine	52 [NA]	42 0.345	0.520	28.366	0.644	37	105	42	100	120	7 duplicate
14988	69 Arginine	43 [548; Leucine (2TBS)]	57 0.333	0.537	16.616	0.480	38	104	40	102	39	104 duplicate
12481	69 Arginine	20 [619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	31 0.303	0.730	27.987	0.654	39	103	22	120	116	5 duplicate
7354	69 Arginine	108 Octadecenoic acid	60 0.295	0.419	21.325	0.381	40	102	44	98	68	133 original
16811	69 Arginine	33 Glutamine	48 0.282	0.588	20.342	0.628	41	101	36	108	61	16 duplicate
14281	69 Arginine	66 [596; N-Acetylglutamic acid (2TMS)]	60 0.268	0.538	13.470	0.512	42	100	39	103	19	86 duplicate
7321	69 Arginine	75 Lysine	60 0.267	0.582	23.312	0.515	43	99	37	105	85	83 original
16411	69 Arginine	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	60 0.218	0.525	10.208	0.505	44	98	41	101	7	90 duplicate
7317	69 Arginine	71 [731; Erythrose (3TMS)]	60 0.181	0.197	13.150	0.485	45	97	49	93	18	102 original
7365	69 Arginine	119 [931; myo-Inositol-2-phosphate (7TMS)]	60 0.149	0.097	18.631	0.493	46	96	53	89	50	97 original
7370	69 Arginine	124 [734; 1-Monodeoxyglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	55 0.131	0.291	36.982	0.414	47	95	46	98	140	129 original
7353	69 Arginine	107 9-(Z)-Octadecenoic acid	60 0.123	0.180	12.179	0.403	48	94	50	92	14	130 original
7383	69 Arginine	137 Ergosterol	60 0.064	0.120	14.891	0.443	49	93	51	91	28	119 original
7376	69 Arginine	130 Trehalose	59 0.063	0.222	15.870	0.391	50	92	48	94	35	132 original
7385	69 Arginine	139 [700; Ergosta-5,7-dien-3-ol]	35 0.052	0.098	27.667	0.370	51	91	52	90	113	134 original
7384	69 Arginine	138 [674; Ergosterol (1TMS)]	43 0.037	0.048	27.267	0.435	52	90	55	87	112	123 original
10425	69 Arginine	4 Phosphoric acid	49 0.034	0.339	16.859	0.418	53	89	45	97	41	127 duplicate
7318	69 Arginine	72 [919; D-Xylopyranose (4TMS)]	60 0.031	0.086	23.192	0.359	54	88	54	88	83	135 original
15913	69 Arginine	53 Glycerol-2-phosphate	60 -0.014	-0.005	26.663	0.335	55	87	57	85	104	140 duplicate
7339	69 Arginine	93 [607; Putrescine (4TMS)]	56 -0.017	-0.287	31.795	0.470	56	86	67	75	131	109 original
7336	69 Arginine	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	60 -0.020	-0.078	18.632	0.337	57	85	58	84	51	139 original
7387	69 Arginine	141 Lanosta-8,24-dien-3-beta-ol	58 -0.024	-0.118	23.782	0.464	58	84	59	83	127	114 original
7330	69 Arginine	84 Mannitol	58 -0.032	-0.483	21.010	0.504	59	83	78	68	66	91 original
11868	69 Arginine	15 Alanine	60 -0.035	-0.173	14.505	0.603	60	82	62	80	24	32 duplicate
16888	69 Arginine	64 [789; Tyramine (3TMS)]	59 -0.060	-0.134	20.475	0.338	61	81	60	82	62	138 duplicate
7357	69 Arginine	111 [583; Erythritol (4TMS)]	39 -0.066	-0.198	29.152	0.341	62	80	63	79	123	137 original
7379	69 Arginine	133 [855; Squalene]	60 -0.093	0.007	19.294	0.394	63	79	58	86	54	131 original
7364	69 Arginine	118 [828; Glucopyranose-6-phosphate (6TMS)]	54 -0.094	-0.164	22.279	0.354	64	78	61	81	78	136 original
7373	69 Arginine	127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	35 -0.106	-0.495	12.776	0.536	65	77	77	65	16	65 original
7340	69 Arginine	94 Hexadecanoic acid	60 -0.110	-0.294	16.027	0.442	66	76	68	74	37	120 original

7355	69 Arginine	109	Octadecanoic acid	60	-0.115	-0.375	18.996	0.483	67	75	71	58	116	original
7386	69 Arginine	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	46	-0.123	-0.283	29.612	0.472	68	74	68	76	128	108 original
7329	69 Arginine	83	Sorbitol	55	-0.126	0.271	10.776	0.462	69	73	47	85	9	117 original
7325	69 Arginine	79	Glucose	60	-0.134	-0.387	22.366	0.517	70	72	72	70	79	76 original
15370	69 Arginine	47	[NA]	60	-0.200	-0.219	22.934	0.468	71	71	65	77	81	113 duplicate
7342	69 Arginine	96	myo-Inositol	47	-0.203	-0.219	33.354	0.305	72	70	64	78	134	141 original
7369	69 Arginine	123	[945; Galactoturanose-6-phosphate (7TMS)]	60	-0.217	-0.346	16.014	0.519	73	69	73	38	71	original
7381	69 Arginine	135	[902; Melibiose (8TMS); alpha-D-Gal-(1,8)-D-Glc (8TMS)]	60	-0.225	-0.517	14.134	0.516	74	68	78	64	20	78 original
7378	69 Arginine	132	[895; Isomaltose methoxyamine (8TMS)]	38	-0.232	-0.816	26.803	0.517	75	67	115	27	107	75 original
7362	69 Arginine	116	[892; Pseudouridine (5TMS)]	30	-0.260	-0.348	18.711	0.420	76	66	70	72	57	126 original
7360	69 Arginine	114	Fructose-6-phosphate	49	-0.287	-0.575	23.381	0.520	77	65	85	57	86	70 original
7374	69 Arginine	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	41	-0.288	-0.604	15.454	0.474	78	64	92	50	30	106 original
7359	69 Arginine	113	Galactose-6-phosphate	58	-0.304	-0.576	25.249	0.493	79	63	86	56	98	98 original
7358	69 Arginine	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (8TMS)]	59	-0.308	-0.597	32.365	0.518	80	62	90	52	133	74 original
7348	69 Arginine	102	[904; Galactose methoxyamine (5TMS)]	60	-0.328	-0.595	23.100	0.516	81	61	89	53	82	80 original
10011	69 Arginine	1	[938; Sulfuric acid (2TMS)]	32	-0.335	-0.602	14.215	0.539	82	60	91	51	22	64 duplicate
7331	69 Arginine	85	[529; Methylenic acid (4TMS)]	48	-0.339	-0.653	20.564	0.511	83	59	96	46	63	88 original
12238	69 Arginine	18	[590; 1-Acetyl-2-thiohydantoin]	60	-0.341	-0.563	18.775	0.475	84	58	83	59	52	112 duplicate
14781	69 Arginine	41	[639; Proline (2TMS)]	60	-0.344	-0.411	15.417	0.467	85	57	73	69	29	105 duplicate
7350	69 Arginine	104	[795; Erythritol (4TMS)]	60	-0.356	-0.472	21.967	0.484	86	56	75	67	74	103 original
7337	69 Arginine	91	[766; beta-D-Methylglucopyranoside (4TMS)]	60	-0.362	-0.591	27.824	0.463	87	55	88	54	114	115 original
7348	69 Arginine	100	[857; Mannitol (8TMS)]	60	-0.365	-0.689	18.139	0.541	88	54	100	42	47	63 original
7372	69 Arginine	126	[559; Erythritol (4TMS)]	41	-0.366	-0.537	17.821	0.597	89	53	80	62	43	34 original
7320	69 Arginine	74	[912; Tetradecanoic acid (1TMS)]	60	-0.366	-0.570	25.811	0.523	90	52	84	58	101	69 original
7326	69 Arginine	80	[772; D-Glucose (5TMS)]	58	-0.376	-0.539	22.168	0.441	91	51	81	61	76	121 original
7366	69 Arginine	120	[845; Uridine (3TMS)]	50	-0.388	-0.419	14.204	0.620	92	50	74	68	21	19 original
12360	69 Arginine	19	Alanine (BP) (3TMS)	60	-0.398	-0.542	17.990	0.488	93	49	82	60	46	100 duplicate
7343	69 Arginine	97	[756; beta-D-Methylglucopyranoside (4TMS)]	48	-0.399	-0.665	21.890	0.492	94	48	98	44	71	99 original
10696	69 Arginine	6	Glycerol	60	-0.411	-0.610	26.664	0.437	95	47	93	49	105	122 duplicate
7347	69 Arginine	101	[832; Dopamine (4TMS)]	60	-0.441	-0.644	23.804	0.469	97	45	95	47	91	110 original
14176	69 Arginine	35	Pyroglutamic acid	60	-0.446	-0.729	26.832	0.571	98	44	104	38	108	50 duplicate
11485	69 Arginine	12	Glycercic acid	59	-0.454	-0.828	28.125	0.566	99	43	118	24	118	54 duplicate
7345	69 Arginine	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	37	-0.465	-0.878	21.224	0.581	100	42	128	14	67	43 original
7361	69 Arginine	115	Glucose-6-phosphate	58	-0.471	-0.709	17.971	0.552	101	41	102	40	45	57 original
15085	69 Arginine	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	46	-0.474	-0.705	19.465	0.495	102	40	101	41	56	84 duplicate
13186	69 Arginine	26	Citramalic acid	60	-0.485	-0.780	13.094	0.535	103	39	111	31	17	67 duplicate
7338	69 Arginine	92	[680; Glycerol-2-phosphate (4TMS)]	50	-0.486	-0.629	21.494	0.449	104	38	94	48	70	118 original
7333	69 Arginine	87	[945; beta-D-Glucopyranose (5TMS)]	59	-0.493	-0.656	25.668	0.473	105	37	97	45	99	107 original
12601	69 Arginine	105	[705; 2-Ketogluconic acid (5TMS)]	44	-0.495	-0.747	19.071	0.494	106	36	107	35	53	95 original
7351	69 Arginine	21	[678; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	60	-0.499	-0.763	15.104	0.570	107	35	113	29	27	51 duplicate
7371	69 Arginine	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	60	-0.501	-0.689	23.394	0.519	108	34	99	43	88	73 original
7349	69 Arginine	103	[848; Ethylamine (2TMS)]	59	-0.508	-0.733	25.671	0.507	109	33	106	36	100	89 original
12720	69 Arginine	22	[690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	50	-0.517	-0.857	28.020	0.581	110	32	125	17	117	42 duplicate
7363	69 Arginine	117	[724; Glycerol (3TMS)]	52	-0.517	-0.748	23.389	0.555	111	31	108	34	87	56 original
13413	69 Arginine	28	Malic acid	60	-0.519	-0.870	17.949	0.610	112	30	126	16	44	29 duplicate
7367	69 Arginine	121	[657; Erythritol (4TMS)]	51	-0.520	-0.710	28.368	0.513	113	29	103	39	121	84 original
7324	69 Arginine	78	Mannose	58	-0.537	-0.729	28.228	0.511	114	28	105	37	119	87 original
14891	69 Arginine	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	60	-0.540	-0.827	20.211	0.596	115	27	117	25	59	36 duplicate
7356	69 Arginine	110	[715; Erythritol (4TMS)]	50	-0.541	-0.760	26.115	0.596	116	26	109	33	102	37 original
11740	69 Arginine	14	Fumaric acid	60	-0.546	-0.875	26.463	0.616	117	25	127	15	103	24 duplicate

14488	69 Arginine	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	60	-0.553	-0.896	20.568	0.608	118	24	133	9	65	31 duplicate
7368	69 Arginine	122	[644; Erythritol (4TMS)]	48	-0.553	-0.798	28.938	0.566	119	23	114	28	122	52 original
11356	69 Arginine	11	Succinic acid	60	-0.562	-0.838	19.422	0.574	120	22	120	22	55	47 duplicate
13525	69 Arginine	29	Erythritol	60	-0.569	-0.896	21.929	0.629	121	21	131	11	73	15 duplicate
7319	69 Arginine	73	[708; Glucose methoxyamine (5TMS)]	54	-0.572	-0.763	27.204	0.551	123	19	121	21	111	59 original
16000	69 Arginine	54	[NA]	51	-0.586	-0.841	27.243	0.517	123	19	121	21	111	77 duplicate
12115	69 Arginine	17	[700; 2-methyl-1,2-propanediol (2TMS)]	60	-0.589	-0.848	18.606	0.576	124	18	122	20	49	45 duplicate
7316	69 Arginine	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	54	-0.589	-0.524	15.597	0.425	125	17	79	63	33	125 original
7322	69 Arginine	76	Fructose	60	-0.592	-0.782	21.929	0.573	126	16	112	30	72	48 original
7352	69 Arginine	106	[733; Threitol (4TMS)]	58	-0.600	-0.818	23.899	0.613	127	15	116	26	94	27 original
7334	69 Arginine	88	Glucuronic acid	60	-0.611	-0.850	22.500	0.624	128	14	123	19	80	18 original
16733	69 Arginine	62	[812; D-Xylofuranose (4TMS)]	60	-0.614	-0.836	15.557	0.593	128	13	119	23	32	40 duplicate
7380	69 Arginine	134	Isomaltose	60	-0.617	-0.904	24.728	0.649	130	12	136	6	96	6 original
7332	69 Arginine	86	[793; D-Galactono-1,4-lactone (4TMS)]	59	-0.624	-0.854	29.578	0.636	131	11	124	18	125	13 original
12955	69 Arginine	24	[725; 2-Ketooctanoic acid (2TMS)]	60	-0.633	-0.927	22.221	0.655	132	10	138	4	77	3 duplicate
11991	69 Arginine	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	60	-0.640	-0.928	17.485	0.627	133	9	139	3	42	17 duplicate
16328	69 Arginine	57	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	51	-0.641	-0.879	25.052	0.598	134	8	129	13	97	33 duplicate
15276	69 Arginine	46	Arabinose	60	-0.643	-0.887	26.938	0.643	135	6	130	12	109	8 duplicate
16244	69 Arginine	58	[828; Orotic acid (3TMS)]	60	-0.643	-0.899	28.489	0.634	136	7	134	8	124	14 duplicate
14590	69 Arginine	39	[829; 1-Phenylethanol (1TMS)]	59	-0.643	-0.922	24.497	0.619	137	5	137	5	95	22 duplicate
16964	69 Arginine	65	[646; 3-Deoxyglucitol (5TMS)]	59	-0.654	-0.903	31.213	0.640	138	4	135	7	130	10 duplicate
7375	69 Arginine	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	55	-0.658	-0.896	26.786	0.575	139	3	132	10	106	48 original
11613	69 Arginine	13	Uracil	60	-0.690	-0.937	20.308	0.640	140	2	141	1	60	9 duplicate
15946	69 Arginine	50	[746; Ribonic acid-1,4-lactone (3TMS)]	57	-0.702	-0.934	35.230	0.610	141	1	140	2	137	30 duplicate
16734	70 [693; 2-Furan-2-hydroxy	62	[812; D-Xylofuranose (4TMS)]	57	0.620	0.648	7.464	0.471	1	141	18	124	6	48 duplicate
11992	70 [693; 2-Furan-2-hydroxy	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	57	0.602	0.581	6.453	0.497	2	140	27	115	1	35 duplicate
15647	70 [693; 2-Furan-2-hydroxy	50	[746; Ribonic acid-1,4-lactone (3TMS)]	54	0.596	0.549	31.298	0.445	3	139	39	103	136	66 duplicate
11614	70 [693; 2-Furan-2-hydroxy	13	Uracil	57	0.591	0.591	8.476	0.551	4	138	24	118	9	4 duplicate
16965	70 [693; 2-Furan-2-hydroxy	65	[646; 3-Deoxyglucitol (5TMS)]	56	0.590	0.646	21.532	0.521	5	137	19	123	102	28 duplicate
7383	70 [693; 2-Furan-2-hydroxy	76	Fructose	57	0.584	0.754	8.768	0.549	6	135	1	141	10	5 original
7451	70 [693; 2-Furan-2-hydroxy	134	Isomaltose	57	0.584	0.654	10.731	0.544	7	136	16	128	23	7 original
12958	70 [693; 2-Furan-2-hydroxy	24	[725; 2-Ketooctanoic acid (2TMS)]	57	0.570	0.607	13.727	0.527	8	134	21	121	35	18 duplicate
13414	70 [693; 2-Furan-2-hydroxy	28	Malic acid	57	0.569	0.581	11.645	0.457	9	133	26	116	25	60 duplicate
15277	70 [693; 2-Furan-2-hydroxy	46	Arabinose	57	0.566	0.671	13.933	0.523	10	132	10	132	39	23 duplicate
7432	70 [693; 2-Furan-2-hydroxy	115	Glucose-6-phosphate	55	0.566	0.731	7.495	0.472	11	131	3	139	7	47 original
14591	70 [693; 2-Furan-2-hydroxy	39	[829; 1-Phenylethanol (1TMS)]	56	0.560	0.576	12.347	0.488	12	130	29	113	28	42 duplicate
7446	70 [693; 2-Furan-2-hydroxy	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	52	0.560	0.594	18.625	0.509	13	129	23	119	79	31 original
14489	70 [693; 2-Furan-2-hydroxy	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	57	0.559	0.580	13.832	0.439	14	128	28	114	36	70 duplicate
11357	70 [693; 2-Furan-2-hydroxy	11	Succinic acid	57	0.554	0.563	13.451	0.431	15	126	33	109	33	74 duplicate
11741	70 [693; 2-Furan-2-hydroxy	14	Fumaric acid	57	0.554	0.555	21.808	0.428	16	127	36	106	103	75 duplicate
7423	70 [693; 2-Furan-2-hydroxy	106	[733; Threitol (4TMS)]	55	0.550	0.682	14.041	0.531	17	125	8	134	40	15 original
12602	70 [693; 2-Furan-2-hydroxy	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	57	0.550	0.500	6.695	0.440	18	124	48	94	2	69 duplicate
7395	70 [693; 2-Furan-2-hydroxy	78	Mannose	56	0.549	0.659	20.891	0.467	19	123	14	128	98	51 original
16245	70 [693; 2-Furan-2-hydroxy	56	[829; Orotic acid (3TMS)]	57	0.546	0.661	20.841	0.523	20	122	13	129	97	22 duplicate
13528	70 [693; 2-Furan-2-hydroxy	40	[690; 2,3-Dimethylsuccinic acid (2TMS)]	57	0.540	0.559	17.058	0.406	21	121	35	107	65	87 duplicate
14692	70 [693; 2-Furan-2-hydroxy	40	[690; 2,3-Dimethylsuccinic acid (2TMS)]	57	0.536	0.572	16.923	0.468	22	120	30	112	64	49 duplicate
14177	70 [693; 2-Furan-2-hydroxy	35	Pyroglutamic acid	57	0.530	0.725	22.340	0.525	23	118	5	137	104	20 duplicate
12116	70 [693; 2-Furan-2-hydroxy	17	[700; 2-methyl-1,2-propanediol (2TMS)]	57	0.530	0.559	7.435	0.468	24	119	34	108	5	50 duplicate

7403	70	[693; 2-Furan-2-hydroxy	86	[793; D-Galactono-1,4-lactone (4TMS)]	54	0.529	0.671	15.435	0.517	25	117	9	133	51	28 original
12721	70	[693; 2-Furan-2-hydroxy	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	45	0.515	0.416	23.551	0.417	26	116	58	84	109	80 duplicate
7442	70	[693; 2-Furan-2-hydroxy	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	57	0.511	0.732	13.196	0.532	27	115	2	140	31	12 original
16001	70	[693; 2-Furan-2-hydroxy	54	[NA]	48	0.511	0.521	23.821	0.491	28	114	46	96	111	39 duplicate
7405	70	[693; 2-Furan-2-hydroxy	88	Gluconic acid	57	0.509	0.545	12.989	0.489	29	113	40	102	30	40 original
	70	[693; 2-Furan-2-hydroxy													
16329	57	[757; 2-Desoxy-pentos-3-yose dimethoxyamine (2TMS)]	57		48	0.500	0.582	16.055	0.525	30	111	25	117	57	21 duplicate
7438	70	[693; 2-Furan-2-hydroxy	121	[657; Erythritol (4TMS)]	48	0.500	0.555	25.351	0.526	31	112	37	105	117	19 original
7390	70	[693; 2-Furan-2-hydroxy	73	[708; Glucose methoxyamine (5TMS)]	54	0.497	0.720	19.798	0.493	32	110	7	135	91	37 original
7430	70	[693; 2-Furan-2-hydroxy	113	Galactose-6-phosphate	55	0.492	0.725	19.305	0.523	34	108	4	138	86	24 original
7409	70	[693; 2-Furan-2-hydroxy	92	[680; Glycerol-2-phosphate (4TMS)]	57	0.498	0.611	17.570	0.514	35	107	20	122	71	30 original
7434	70	[693; 2-Furan-2-hydroxy	117	[724; Glycerol (3TMS)]	40	0.474	0.526	18.365	0.472	36	106	45	97	77	46 original
12361	70	[693; 2-Furan-2-hydroxy	19	Alanine (BP) (3TMS)	57	0.472	0.651	9.787	0.489	37	105	17	125	14	41 duplicate
7420	70	[693; 2-Furan-2-hydroxy	103	[848; Ethylamine (2TMS)]	56	0.465	0.518	16.227	0.463	38	104	47	95	58	54 original
7431	70	[693; 2-Furan-2-hydroxy	114	Fructose-6-phosphate	46	0.463	0.722	18.751	0.517	39	103	6	136	80	27 original
7417	70	[693; 2-Furan-2-hydroxy	100	[857; Mannitol (6TMS)]	57	0.457	0.475	12.334	0.341	40	102	51	91	27	134 original
7427	70	[693; 2-Furan-2-hydroxy	110	[715; Erythritol (4TMS)]	47	0.449	0.539	21.503	0.521	41	101	42	100	101	25 original
7439	70	[693; 2-Furan-2-hydroxy	122	[844; Erythritol (4TMS)]	45	0.442	0.454	26.891	0.534	42	100	56	86	123	11 original
13187	70	[693; 2-Furan-2-hydroxy	26	Citramalic acid	57	0.440	0.454	6.977	0.449	43	99	52	90	4	63 duplicate
7437	70	[693; 2-Furan-2-hydroxy	120	[945; Uridine (3TMS)]	48	0.436	0.214	10.148	0.401	44	98	71	71	21	92 original
7402	70	[693; 2-Furan-2-hydroxy	85	[528; Methylcitric acid (4TMS)]	46	0.432	0.535	14.145	0.357	45	97	43	99	42	130 original
7440	70	[693; 2-Furan-2-hydroxy	123	[945; Galactofuranose-6-phosphate (7TMS)]	57	0.429	0.668	9.886	0.508	46	98	11	131	17	32 original
11486	70	[693; 2-Furan-2-hydroxy	12	Glyceric acid	56	0.414	0.420	23.956	0.390	47	95	57	85	113	105 duplicate
14782	70	[693; 2-Furan-2-hydroxy	41	[639; Proline (2TMS)]	57	0.401	0.533	8.192	0.464	48	94	44	98	8	53 duplicate
7418	70	[693; 2-Furan-2-hydroxy	101	[832; Dopamine (4TMS)]	57	0.398	0.475	16.228	0.424	49	93	50	92	59	77 original
7419	70	[693; 2-Furan-2-hydroxy	102	[804; Galactose methoxyamine (5TMS)]	57	0.397	0.444	18.884	0.363	50	92	53	89	83	123 original
12239	70	[693; 2-Furan-2-hydroxy	18	[590; 1-Acetyl-2-thiohydantoin]	57	0.380	0.442	13.554	0.397	51	91	54			



7428	70 [693; 2-Furan-2-hydroxy 111 [583; Erythritol (4TMS)]	36	0.178	0.311	29.866	0.459	75	67	65	77	133	58 original
7444	70 [693; 2-Furan-2-hydroxy 127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	33	0.170	0.053	15.585	0.447	76	66	79	63	52	65 original
7435	70 [693; 2-Furan-2-hydroxy 118 [928; Glucopyranose-6-phosphate (6TMS)]	51	0.153	0.293	19.710	0.413	77	65	67	75	90	81 original
7457	70 [693; 2-Furan-2-hydroxy 140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	46	0.144	0.084	26.653	0.300	78	64	78	64	122	138 original
7455	70 [693; 2-Furan-2-hydroxy 138 [674; Ergosterol (1TMS)]	43	0.141	0.170	26.974	0.305	79	63	75	67	124	137 original
7426	70 [693; 2-Furan-2-hydroxy 109 Octadecanoic acid	57	0.085	0.207	12.310	0.462	80	62	66	76	26	56 original
7411	70 [693; 2-Furan-2-hydroxy 94 Hexadecanoic acid	57	0.051	0.213	9.876	0.410	81	61	72	70	16	84 original
15371	70 [693; 2-Furan-2-hydroxy 47 [NA]	57	0.046	-0.014	19.451	0.317	82	60	82	60	87	136 duplicate
7388	70 [693; 2-Furan-2-hydroxy 71 [731; Erythrose (3TMS)]	57	0.011	0.031	9.792	0.369	83	59	81	61	15	121 original
7458	70 [693; 2-Furan-2-hydroxy 141 Lanosta-8,24-dien-3-ol	55	0.007	-0.112	25.959	0.358	84	58	90	52	120	127 original
7456	70 [693; 2-Furan-2-hydroxy 139 [700; Ergosta-5,7-dien-3-ol]	35	-0.035	-0.215	27.484	0.280	85	57	97	45	125	141 original
16412	70 [693; 2-Furan-2-hydroxy [636; 4R-Acetalido-2,3-(Z)-epoxy-4(E)-hydroxycyclohexane (1TMS)]	57	-0.044	-0.034	10.655	0.374	86	56	86	56	22	116 duplicate
7401	70 [693; 2-Furan-2-hydroxy 84 Mannitol	55	-0.052	-0.023	16.291	0.389	87	55	84	58	61	107 original
10426	70 [693; 2-Furan-2-hydroxy 4 Phosphoric acid	48	-0.057	-0.163	18.237	0.350	88	54	92	60	75	132 duplicate
7392	70 [693; 2-Furan-2-hydroxy 75 Lysine	57	-0.060	-0.016	22.869	0.411	89	53	83	59	105	82 original
7389	70 [693; 2-Furan-2-hydroxy 72 [918; D-Xylopyranose (4TMS)]	57	-0.061	-0.148	21.158	0.336	90	52	91	51	99	135 original
14282	70 [693; 2-Furan-2-hydroxy 36 [596; N-Acetylglutamic acid (2TMS)]	57	-0.070	-0.092	14.301	0.386	91	51	88	54	45	110 duplicate
7454	70 [693; 2-Furan-2-hydroxy 137 Ergosterol	57	-0.076	-0.258	14.242	0.373	92	50	99	43	44	117 original
7441	70 [693; 2-Furan-2-hydroxy 124 [734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]	53	-0.094	-0.189	34.976	0.395	93	49	83	49	140	100 original
7447	70 [693; 2-Furan-2-hydroxy 130 Trehalose	56	-0.130	-0.024	13.844	0.347	94	48	85	57	38	133 original
15914	70 [693; 2-Furan-2-hydroxy 53 Glycerol-2-phosphate	57	-0.152	-0.263	24.289	0.352	95	47	100	42	114	131 duplicate
7410	70 [693; 2-Furan-2-hydroxy 93 [607; Putrescine (4TMS)]	53	-0.154	-0.053	28.727	0.358	96	46	87	55	128	128 original
7436	70 [693; 2-Furan-2-hydroxy 119 [931; myo-Inositol-2-phosphate (7TMS)]	57	-0.182	-0.383	16.811	0.390	97	45	110	32	63	106 original
7407	70 [693; 2-Furan-2-hydroxy 90 [910; 9-(Z)-Hexadecanoic acid (1TMS)]	57	-0.194	-0.376	15.818	0.397	98	44	108	34	56	98 original
10831	70 [693; 2-Furan-2-hydroxy 7 Threonine	57	-0.197	-0.186	14.513	0.399	99	43	94	48	47	96 duplicate
7453	70 [693; 2-Furan-2-hydroxy 136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	16	-0.200	-0.343	11.090	0.418	100	42	106	38	24	79 original
13301	70 [693; 2-Furan-2-hydroxy 27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	48	-0.245	-0.329	27.952	0.361	101	41	105	37	126	124 duplicate
17040	70 [693; 2-Furan-2-hydroxy 66 Glyceral acid-3-phosphate	57	-0.247	-0.249	19.120	0.387	102	40	98	44	84	108 duplicate
14989	70 [693; 2-Furan-2-hydroxy 43 [548; Leucine (2TBS)]	53	-0.253	-0.291	15.095	0.373	103	39	101	41	49	118 duplicate
10151	70 [693; 2-Furan-2-hydroxy 2 Serine	56	-0.260	-0.211	14.420	0.410	104	38	86	46	46	85 duplicate
7424	70 [693; 2-Furan-2-hydroxy 107 9-(Z)-Octadecanoic acid	57	-0.264	-0.490	10.126	0.395	105	37	122	20	20	101 original
7415	70 [693; 2-Furan-2-hydroxy 98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	42	-0.282	-0.539	28.964	0.400	106	36	126	16	130	94 original
16575	70 [693; 2-Furan-2-hydroxy 60 Glycerol-3-phosphate	57	-0.313	-0.364	9.835	0.392	107	35	107	35	18	104 duplicate
13072	70 [693; 2-Furan-2-hydroxy 25 [709; 2,5-Diaminovalerolactam (2TMS)]	41	-0.332	-0.324	24.857	0.515	108	34	104	38	116	29 duplicate
7425	70 [693; 2-Furan-2-hydroxy 108 Octadecanoic acid	57	-0.342	-0.458	20.100	0.401	109	33	121	21	92	90 original
17114	70 [693; 2-Furan-2-hydroxy 67 Citric acid	57	-0.346	-0.389	9.935	0.402	110	32	112	30	19	89 duplicate
15926	70 [693; 2-Furan-2-hydroxy 52 [NA]	40	-0.367	-0.670	28.868	0.442	111	31	135	7	129	67 duplicate
14386	70 [693; 2-Furan-2-hydroxy 37 Phenylalanine	57	-0.373	-0.376	9.746	0.405	112	30	109	33	13	88 duplicate
12839	70 [693; 2-Furan-2-hydroxy 23 Homoserine	57	-0.378	-0.505	18.775	0.409	113	29	123	19	81	86 duplicate
17187	70 [693; 2-Furan-2-hydroxy 68 [570; Hypoxanthine (2TMS)]	18	-0.386	-0.830	18.179	0.359	114	28	137	5	74	128 duplicate
11096	70 [693; 2-Furan-2-hydroxy 9 Proline	56	-0.392	-0.198	17.530	0.431	115	27	95	47	70	73 duplicate
15182	70 [693; 2-Furan-2-hydroxy 45 Homocysteine	54	-0.399	-0.406	33.587	0.358	116	26	115	27	139	129 duplicate
13747	70 [693; 2-Furan-2-hydroxy 31 [622; Parabenic acid (2TMS)]	57	-0.411	-0.390	23.628	0.383	117	25	113	29	110	113 duplicate
10964	70 [693; 2-Furan-2-hydroxy 8 Isoleucine	51	-0.412	-0.322	12.909	0.384	118	24	103	39	29	112 duplicate
16812	70 [693; 2-Furan-2-hydroxy 63 Glutamine	46	-0.422	-0.707	25.575	0.491	119	23	136	6	118	38 duplicate
13856	70 [693; 2-Furan-2-hydroxy 32 [728; N,N-Dimethyllysine methyl ester]	57	-0.442	-0.385	26.274	0.394	120	22	111	31	121	102 duplicate
16655	70 [693; 2-Furan-2-hydroxy 61 [NA]	57	-0.444	-0.512	17.292	0.449	121	21	124	18	68	82 duplicate
14071	70 [693; 2-Furan-2-hydroxy 34 Aspartic acid	57	-0.479	-0.404	18.426	0.387	122	20	114	28	78	109 duplicate
10289	70 [693; 2-Furan-2-hydroxy 3 Ethanolamine	56	-0.480	-0.549	23.879	0.532	123	19	127	15	112	133 duplicate

7412	70 [693; 2-Furan-2-hydroxy	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	45	-0.495	-0.424	29,108	0.457	124	18	118	24	131	59 original
15556	70 [693; 2-Furan-2-hydroxy	49	[877; Pyrophosphoric acid (4TMS)]	57	-0.503	-0.551	32,781	0.451	125	17	128	14	138	61 duplicate
7448	70 [693; 2-Furan-2-hydroxy	131	[626; 5-Methylthiodenosine (3TMS)]	48	-0.516	-0.607	28,272	0.537	126	16	132	10	127	10 original
15464	70 [693; 2-Furan-2-hydroxy	48	Asparagine	57	-0.516	-0.668	20,801	0.498	127	15	133	9	96	34 duplicate
13964	70 [693; 2-Furan-2-hydroxy	33	Methionine	57	-0.528	-0.425	18,296	0.401	128	14	119	23	76	91 duplicate
11227	70 [693; 2-Furan-2-hydroxy	30	Glycine	57	-0.553	-0.601	13,281	0.531	129	13	131	11	32	14 duplicate
13637	70 [693; 2-Furan-2-hydroxy	30	[815; Ethyl-3(2H)-thiophenone]	57	-0.555	-0.415	17,937	0.400	130	12	117	25	73	85 duplicate
16494	70 [693; 2-Furan-2-hydroxy	59	Omithine; Arginine	57	-0.561	-0.408	24,548	0.394	131	11	116	26	115	103 duplicate
15737	70 [693; 2-Furan-2-hydroxy	51	[498; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	42	-0.568	-0.669	30,514	0.399	132	10	134	8	134	97 duplicate
7394	70 [693; 2-Furan-2-hydroxy	77	[826; beta-[[[5-methyl-2-ethenyl)methyl]eneamino- benzeneacetic acid methyl ester]	56	-0.578	-0.428	19,216	0.440	133	9	120	22	85	68 original
16087	70 [693; 2-Furan-2-hydroxy	55	[612; 4-Aminobutyric acid (2TBS)]	41	-0.578	-0.901	32,549	0.541	134	8	140	2	137	9 duplicate
10562	70 [693; 2-Furan-2-hydroxy	5	Leucine	44	-0.588	-0.566	20,175	0.359	135	7	129	13	93	125 duplicate
17259	70 [693; 2-Furan-2-hydroxy	69	Arginine	54	-0.589	-0.524	15,597	0.425	136	6	125	17	53	76 duplicate
7398	70 [693; 2-Furan-2-hydroxy	81	Tyrosine	57	-0.591	-0.576	21,462	0.545	137	5	130	12	100	6 original
12482	70 [693; 2-Furan-2-hydroxy	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	30	-0.600	-0.895	22,995	0.461	138	4	139	3	107	57 duplicate
14891	70 [693; 2-Furan-2-hydroxy	42	Glutamic acid	54	-0.600	-0.321	20,321	0.369	139	3	102	40	95	120 duplicate
7406	70 [693; 2-Furan-2-hydroxy	89	[775; Dopamine (4TMS)]	32	-0.633	-0.911	23,524	0.437	140	2	141	1	108	71 original
7399	70 [693; 2-Furan-2-hydroxy	82	Lysine	38	-0.730	-0.884	17,065	0.528	141	1	138	4	68	17 original
7470	71 [731; Erythrose (3TMS)]	83	Sorbitol	58	0.614	0.677	10,958	0.451	1	141	4	138	37	58 original
17115	71 [731; Erythrose (3TMS)]	67	Citric acid	64	0.592	0.809	12,636	0.507	2	140	1	141	52	12 duplicate
16576	71 [731; Erythrose (3TMS)]	60	Glycerol-3-phosphate	64	0.570	0.780	10,259	0.517	3	139	3	139	31	9 duplicate
7503	71 [731; Erythrose (3TMS)]	116	[882; Pseudouridine (5TMS)]	30	0.545	0.798	12,527	0.503	4	138	2	140	50	13 original
14387	71 [731; Erythrose (3TMS)]	37	Phenylalanine	64	0.494	0.643	11,637	0.458	5	137	7	135	42	49 duplicate
7472	71 [731; Erythrose (3TMS)]	85	[529; Methylcitric acid (4TMS)]	48	0.449	0.656	9,028	0.594	6	136	6	136	22	1 original
7525	71 [731; Erythrose (3TMS)]	139	[674; Ergosterol (1TMS)]	46	0.432	0.580	21,698	0.445	7	135	13	129	109	60 original
10832	71 [731; Erythrose (3TMS)]	94	Threonine	64	0.425	0.669	19,210	0.453	8	134	5	137	98	54 duplicate
7481	71 [731; Erythrose (3TMS)]	94	Hexadecanoic acid	64	0.423	0.613	11,611	0.484	9	133	8	134	41	25 original
10280	71 [731; Erythrose (3TMS)]	3	Ethanolamine	62	0.407	0.560	16,742	0.455	10	132	17	125	79	51 duplicate
7496	71 [731; Erythrose (3TMS)]	109	Octadecanoic acid	64	0.400	0.598	14,062	0.400	11	131	11	131	61	105 original
7524	71 [731; Erythrose (3TMS)]	137	Ergosterol	64	0.393	0.330	8,730	0.382	12	130	35	107	21	122 original
7522	71 [731; Erythrose (3TMS)]	135		64	0.373	0.409	2,141	0.495	13	129	23	119	1	16 original
7528	71 [731; Erythrose (3TMS)]	141	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	61	0.372	0.381	20,250	0.407	14	128	26	116	104	99 original
7468	71 [731; Erythrose (3TMS)]	81	Tyrosine	64	0.359	0.577	23,574	0.479	15	127	14	128	120	27 original
7464	71 [731; Erythrose (3TMS)]	77	[826; beta-[[[5-methyl-2-ethenyl)methyl]eneamino- benzeneacetic acid methyl ester]	62	0.327	0.565	20,027	0.453	16	126	16	128	103	55 original
7513	71 [731; Erythrose (3TMS)]	126	[559; Erythritol (4TMS)]	45	0.319	0.540	11,788	0.538	17	125	19	123	44	5 original
7482	71 [731; Erythrose (3TMS)]	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	0.314	0.376	24,935	0.398	18	124	27	115	127	108 original
7500	71 [731; Erythrose (3TMS)]	113	Galactose-6-phosphate	62	0.296	0.091	14,557	0.502	19	123	72	70	66	14 original
7527	71 [731; Erythrose (3TMS)]	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	49	0.293	0.214	21,819	0.407	20	122	51	91	110	100 original
17188	71 [731; Erythrose (3TMS)]	68	[570; Hypoxanthine (2TMS)]	20	0.284	0.333	18,403	0.419	21	121	34	108	88	87 duplicate
7498	71 [731; Erythrose (3TMS)]	111	[583; Erythritol (4TMS)]	42	0.278	0.348	25,437	0.374	22	120	32	110	129	126 original
14283	71 [731; Erythrose (3TMS)]	36	[596; N-Acetylglutamic acid (2TMS)]	64	0.276	0.599	17,880	0.469	23	119	10	132	85	38 duplicate
7511	71 [731; Erythrose (3TMS)]	124	[734; 1-Monoleoylglycerol (2TMS); 1- Monohexadecanoylglycerol (1TMS)]	59	0.275	0.297	30,220	0.384	24	118	39	103	138	120 original
7501	71 [731; Erythrose (3TMS)]	114	Fructose-6-phosphate	53	0.274	0.135	14,508	0.473	25	117	64	78	65	35 original
7520	71 [731; Erythrose (3TMS)]	133	[855; Squalene]	64	0.273	0.370	9,633	0.416	26	116	29	113	26	91 original
13638	71 [731; Erythrose (3TMS)]	30	[815; Ethyl-3(2H)-thiophenone]	64	0.267	0.409	19,800	0.395	27	115	24	118	100	110 duplicate
17041	71 [731; Erythrose (3TMS)]	66	Glyceric acid-3-phosphate	64	0.265	0.602	11,934	0.471	28	113	9	133	45	36 duplicate

7469	71 [731; Erythrose (3TMS)]	102 [904; Galactose methoxyamine (5TMS)]	64	0.265	0.268	-12.266	0.478	29	114	43	99	47	30 original
16495	71 [731; Erythrose (3TMS)]	59 Ornithine; Arginine	64	0.247	0.537	30.189	0.459	30	112	20	122	137	45 duplicate
7487	71 [731; Erythrose (3TMS)]	100 [857; Mannitol (6TMS)]	64	0.239	0.172	5.731	0.437	31	111	61	81	9	68 original
11228	71 [731; Erythrose (3TMS)]	10 Glycine	64	0.235	0.285	9.753	0.471	32	110	41	101	28	37 duplicate
15738	71 [731; Erythrose (3TMS)]	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	0.228	0.286	25.411	0.485	33	109	40	102	128	23 duplicate
7526	71 [731; Erythrose (3TMS)]	139 [700; Ergosta-5,7-dien-3-ol]	38	0.226	0.110	23.260	0.345	34	108	68	74	118	137 original
11097	71 [731; Erythrose (3TMS)]	9 Proline	63	0.226	0.591	18.911	0.444	35	107	12	130	92	62 duplicate
7461	71 [731; Erythrose (3TMS)]	74 [912; Tetradecanoic acid (1TMS)]	64	0.224	0.424	14.217	0.477	36	108	22	120	62	31 original
7510	71 [731; Erythrose (3TMS)]	123 [945; Galactofuranose-6-phosphate (7TMS)]	64	0.223	0.253	4.523	0.452	37	105	46	96	2	57 original
7523	71 [731; Erythrose (3TMS)]	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.221	0.375	5.630	0.344	38	104	28	114	8	139 original
7483	71 [731; Erythrose (3TMS)]	96 myo-Inositol	49	0.219	0.211	25.801	0.431	39	103	54	88	130	74 original
15087	71 [731; Erythrose (3TMS)]	44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	0.216	0.341	10.454	0.498	40	102	33	108	33	15 duplicate
13965	71 [731; Erythrose (3TMS)]	33 Methionine	64	0.211	0.256	11.440	0.395	41	101	44	98	39	108 duplicate
13748	71 [731; Erythrose (3TMS)]	31 [622; Parabanic acid (2TMS)]	64	0.199	0.353	16.811	0.456	42	100	31	111	80	47 duplicate
14892	71 [731; Erythrose (3TMS)]	42 Glutamic acid	60	0.195	0.368	21.066	0.431	43	99	30	112	108	73 duplicate
7506	71 [731; Erythrose (3TMS)]	119 [931; myo-Inositol-2-phosphate (7TMS)]	64	0.191	0.213	9.147	0.390	44	98	62	90	23	114 original
7499	71 [731; Erythrose (3TMS)]	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.189	0.177	23.597	0.455	45	97	60	82	121	50 original
12240	71 [731; Erythrose (3TMS)]	18 [590; 1-Acetyl-2-thiohydantoin]	64	0.184	0.276	6.847	0.382	46	96	42	100	13	121 duplicate
17260	71 [731; Erythrose (3TMS)]	69 Arginine	60	0.181	0.197	13.150	0.485	47	95	57	85	58	22 duplicate
13857	71 [731; Erythrose (3TMS)]	32 [729; N,N-Dimethyllysine methyl ester]	63	0.175	0.402	20.321	0.477	48	94	25	117	105	32 duplicate
14072	71 [731; Erythrose (3TMS)]	34 Aspartic acid	64	0.165	0.323	22.265	0.382	49	93	37	105	112	123 duplicate
15465	71 [731; Erythrose (3TMS)]	122 [644; Erythritol (4TMS)]	52	0.164	0.227	21.002	0.483	50	92	50	92	107	26 original
15827	71 [731; Erythrose (3TMS)]	52 [NA]	64	0.162	0.203	12.694	0.438	51	91	56	86	53	65 duplicate
7508	71 [731; Erythrose (3TMS)]	121 [657; Erythritol (4TMS)]	46	0.157	0.162	24.008	0.454	52	90	62	80	124	52 duplicate
7460	71 [731; Erythrose (3TMS)]	73 [708; Glucose methoxyamine (5TMS)]	55	0.157	0.298	19.944	0.426	53	89	38	104	102	79 original
7491	71 [731; Erythrose (3TMS)]	104 [795; Erythritol (4TMS)]	57	0.155	0.229	15.528	0.388	54	88	49	93	72	117 original
16556	71 [731; Erythrose (3TMS)]	61 [NA]	63	0.155	0.231	10.735	0.378	55	87	48	94	36	125 original
16088	71 [731; Erythrose (3TMS)]	55 [612; 4-Aminobutyric acid (2TBS)]	64	0.154	0.253	9.331	0.373	56	86	45	97	25	127 duplicate
7519	71 [731; Erythrose (3TMS)]	132 [895; Isomaltose methoxyamine (8TMS)]	43	0.147	0.136	27.751	0.467	57	85	63	79	134	39 duplicate
7497	71 [731; Erythrose (3TMS)]	110 [715; Erythritol (4TMS)]	42	0.136	-0.086	20.406	0.443	58	84	91	51	106	63 original
16890	71 [731; Erythrose (3TMS)]	64 [789; Tyramine (3TMS)]	54	0.126	0.188	16.532	0.531	59	83	58	84	77	6 original
15183	71 [731; Erythrose (3TMS)]	45 Homocysteine	63	0.126	0.123	10.568	0.410	60	82	67	75	35	94 duplicate
14178	71 [731; Erythrose (3TMS)]	35 Pyroglutamic acid	61	0.121	0.037	28.342	0.421	61	81	76	68	135	84 duplicate
16413	71 [731; Erythrose (3TMS)]	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	0.117	-0.030	30.813	0.395	62	80	85	57	139	109 duplicate
7502	71 [731; Erythrose (3TMS)]	115 Glucose-6-phosphate	64	0.107	0.558	7.115	0.452	63	79	18	124	14	56 duplicate
7462	71 [731; Erythrose (3TMS)]	75 Lysine	62	0.106	-0.009	15.025	0.419	64	78	83	59	70	88 original
7485	71 [731; Erythrose (3TMS)]	98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	64	0.106	0.569	28.911	0.461	65	77	15	127	138	44 original
10152	71 [731; Erythrose (3TMS)]	2 Serine	48	0.105	0.069	24.403	0.485	66	76	73	69	125	21 original
14793	71 [731; Erythrose (3TMS)]	41 [639; Proline (2TMS)]	62	0.102	0.469	13.060	0.463	67	75	21	121	57	42 duplicate
12362	71 [731; Erythrose (3TMS)]	19 Alanine (BP) (3TMS)	64	0.093	0.207	5.255	0.437	68	74	55	87	5	67 duplicate
7504	71 [731; Erythrose (3TMS)]	117 [724; Glycerol (3TMS)]	64	0.088	0.130	6.732	0.475	69	73	65	77	12	33 duplicate
10965	71 [731; Erythrose (3TMS)]	8 Isoleucine	56	0.087	0.211	13.023	0.474	70	72	53	89	56	34 original
7495	71 [731; Erythrose (3TMS)]	108 Octadecanoic acid	55	0.086	0.329	12.456	0.453	71	71	36	106	49	53 duplicate
13415	71 [731; Erythrose (3TMS)]	28 Malic acid	64	0.075	0.124	12.827	0.355	72	69	68	76	55	135 original
13188	71 [731; Erythrose (3TMS)]	26 Citramalic acid	64	0.075	-0.005	5.346	0.427	73	70	81	61	6	78 duplicate
14693	71 [731; Erythrose (3TMS)]	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.065	0.053	5.500	0.410	74	68	74	68	7	95 duplicate
7494	71 [731; Erythrose (3TMS)]	107 9-(Z)-Octadecanoic acid	64	0.063	0.089	23.737	0.449	75	67	71	71	123	59 duplicate
12840	71 [731; Erythrose (3TMS)]	23 Homoserine	64	0.061	0.035	4.881	0.392	76	66	77	65	3	113 original
7517	71 [731; Erythrose (3TMS)]	130 Trehalose	64	0.060	0.107	11.447	0.431	77	65	70	72	40	72 duplicate
			63	0.038	0.179	19.187	0.457	78	64	59	83	85	46 original



15648	71 [73]; Erythrose (3TMS)]	50 [746; Ribonic acid-1,4-lactone (3TMS)]	61 -0.245	-0.342	25.920	0.401	128	13	127	15	131	104-juplicate
	128 [940; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]											
7516	71 [73]; Erythrose (3TMS)]	103 [646; Ethylamine (2TMS)]	59 -0.261	-0.311	15.707	0.416	130	12	123	19	73	92 original
7480	71 [73]; Erythrose (3TMS)]	103 [646; Ethylamine (2TMS)]	63 -0.264	-0.436	15.410	0.418	131	11	134	8	71	89 original
11615	71 [73]; Erythrose (3TMS)]	13 Urcil	64 -0.270	-0.319	10.327	0.488	132	10	124	18	32	20-juplicate
7467	71 [73]; Erythrose (3TMS)]	80 [772; D-Glucose (5TMS)]	62 -0.274	-0.344	21.966	0.373	133	9	128	14	111	128 original
15915	71 [73]; Erythrose (3TMS)]	53 Glycero-2-phosphate	64 -0.289	-0.469	17.711	0.372	134	8	135	7	84	129-juplicate
7474	71 [73]; Erythrose (3TMS)]	87 [945; beta-D-Glucopyranose (5TMS)]	62 -0.311	-0.339	26.186	0.430	135	7	126	16	132	75 original
7488	71 [73]; Erythrose (3TMS)]	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41 -0.334	-0.362	15.724	0.422	136	6	129	13	74	83 original
7488	71 [73]; Erythrose (3TMS)]	101 [832; Dopamine (4TMS)]	64 -0.337	-0.515	13.292	0.420	137	5	136	6	59	85 original
7478	71 [73]; Erythrose (3TMS)]	91 [756; beta-D-Methylglucopyranoside (4TMS)]	52 -0.354	-0.559	17.624	0.424	138	4	137	5	83	81 original
10013	71 [73]; Erythrose (3TMS)]	1 [938; Sulfuric acid (2TMS)]	64 -0.397	-0.640	19.217	0.491	139	3	139	3	97	19 original
15372	71 [73]; Erythrose (3TMS)]	47 [NA]	36 -0.422	-0.660	12.067	0.410	140	2	140	2	48	97-juplicate
7574	72 [918; D-Xylopyranose (4 118 [928; Glucopyranose-6-phosphate (6TMS)]		64 -0.493	-0.672	14.309	0.519	141	1	141	1	64	8-juplicate
15373	72 [918; D-Xylopyranose (4 47 [NA]		57 0.474	0.567	6.887	0.409	1	141	2	140	2	11 original
10014	72 [918; D-Xylopyranose (4 1 [938; Sulfuric acid (2TMS)]		63 0.465	0.664	8.389	0.491	2	140	1	141	7	1-juplicate
7536	72 [918; D-Xylopyranose (4 80 [772; D-Glucose (5TMS)]		35 0.371	0.450	6.839	0.444	3	139	3	139	3	3-juplicate
7543	72 [918; D-Xylopyranose (4 87 [945; beta-D-Glucopyranose (5TMS)]		61 0.313	0.296	31.717	0.329	4	138	4	138	123	121 original
15558	72 [918; D-Xylopyranose (4 49 [877; Pyrophosphoric acid (4TMS)]		61 0.219	0.233	36.559	0.377	5	137	6	136	136	38 original
7595	72 [918; D-Xylopyranose (4 139 [700; Ergosta-5,7-dian-3-ol]		63 0.190	0.204	16.713	0.372	6	136	7	135	83	44-juplicate
10428	72 [918; D-Xylopyranose (4 4 Phosphoric acid		37 0.168	0.150	13.679	0.348	7	135	12	130	55	82 original
14784	72 [918; D-Xylopyranose (4 4 [839; Proline (2TMS)]		51 0.156	0.115	34.829	0.354	8	134	19	123	132	78-juplicate
7583	72 [918; D-Xylopyranose (4 127 [777; Fructose-6-phosphate methoxyamine (6TMS)]		63 0.148	0.198	15.635	0.365	9	133	8	134	76	56-juplicate
7538	72 [918; D-Xylopyranose (4 82 Lysine		38 0.141	0.185	7.354	0.335	10	132	10	132	4	109 original
13074	72 [918; D-Xylopyranose (4 25 [709; 2,5-Diaminovalerolactam (2TMS)]		39 0.136	0.270	17.568	0.426	11	131	5	137	89	9 original
7587	72 [918; D-Xylopyranose (4 131 [626; 5-Methylthioadenosine (3TMS)]		47 0.129	0.118	13.510	0.334	12	130	17	125	52	111-juplicate
16814	72 [918; D-Xylopyranose (4 63 Glutamine		54 0.124	0.146	13.100	0.365	13	129	13	129	44	58 original
7555	72 [918; D-Xylopyranose (4 99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]		51 0.112	0.116	14.790	0.318	14	128	18	124	70	129-juplicate
13303	72 [918; D-Xylopyranose (4 27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]		40 0.105	-0.114	10.089	0.395	15	127	70	72	17	17 original
15916	72 [918; D-Xylopyranose (4 53 Glycero-2-phosphate		63 0.075	0.125	16.377	0.314	16	126	16	126	78	133-juplicate
	72 [918; D-Xylopyranose (4 20 [619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]		53 0.069	0.132	8.879	0.330	17	125	14	128	11	118-juplicate
12484	72 [918; D-Xylopyranose (4 55 [612; 4-Aminobutyric acid (2TBS)]		31 0.062	0.108	13.302	0.265	18	124	22	120	46	141-juplicate
16089	72 [918; D-Xylopyranose (4 108 Octadecenoic acid		43 0.059	0.089	18.775	0.317	19	123	24	118	94	131-juplicate
7564	72 [918; D-Xylopyranose (4 84 Mannitol		63 0.056	0.049	8.415	0.329	20	122	27	115	8	122 original
15928	72 [918; D-Xylopyranose (4 52 [NA]		61 0.054	0.109	32.884	0.347	21	121	21	121	129	83 original
7557	72 [918; D-Xylopyranose (4 101 [832; Dopamine (4TMS)]		45 0.051	0.131	16.525	0.293	22	120	15	127	80	139-juplicate
7546	72 [918; D-Xylopyranose (4 90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]		63 0.036	0.042	13.400	0.323	23	118	29	113	50	128 original
15184	72 [918; D-Xylopyranose (4 45 Homocysteine		63 0.036	-0.007	10.060	0.365	24	119	40	102	16	54 original
14991	72 [918; D-Xylopyranose (4 43 [548; Leucine (2TBS)]		60 0.036	0.094	17.891	0.343	25	117	23	119	91	98-juplicate
10564	72 [918; D-Xylopyranose (4 5 Leucine		59 0.036	-0.009	10.338	0.385	26	116	41	101	20	23-juplicate
17261	72 [918; D-Xylopyranose (4 69 Arginine		60 0.031	0.193	9.568	0.394	27	115	9	133	15	18-juplicate
7554	72 [918; D-Xylopyranose (4 98 [697; Ribose-5-phosphate methoxyamine (5TMS)]		48 0.012	0.109	16.402	0.311	28	113	20	122	79	137 original
7566	72 [918; D-Xylopyranose (4 130 Trehalose		62 0.010	0.039	31.951	0.371	30	112	30	112	126	45 original
15466	72 [918; D-Xylopyranose (4 48 Asparagine		63 0.008	0.039	13.352	0.330	31	111	31	111	48	117-juplicate
7568	72 [918; D-Xylopyranose (4 132 [895; Isomaltose methoxyamine (8TMS)]		41 0.007	-0.081	14.700	0.359	32	110	63	79	66	66 original
13958	72 [918; D-Xylopyranose (4 32 [728; N,N-Dimethyllysine methyl ester]		63 0.006	0.032	15.329	0.356	33	109	32	110	72	73-juplicate
7572	72 [918; D-Xylopyranose (4 116 [882; Pseudouridine (5TMS)]		30 0.002	-0.259	10.209	0.428	34	108	120	22	18	8 original
15649	72 [918; D-Xylopyranose (4 50 [746; Ribonic acid-1,4-lactone (3TMS)]		60 0.002	-0.035	15.618	0.343	35	107	51	91	75	96-juplicate
7563	72 [918; D-Xylopyranose (4 107 9-(Z)-Octadecenoic acid		63 0.002	-0.022	16.807	0.400	36	106	46	96	84	15 original

7576	72 [919; D-Xylopyranose (4 120 [945; Uridine (3TMS)]	53	0.001	0.077	14.325	0.347	37	105	26	116	59	84 original
7551	72 [919; D-Xylopyranose (4 95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	0.001	-0.005	17.336	0.350	38	104	39	103	86	81 original
7575	72 [919; D-Xylopyranose (4 119 [931; myo-Inositol-2-phosphate (7TMS)]	48	-0.002	-0.022	10.886	0.339	39	103	47	95	24	102 original
7596	72 [919; D-Xylopyranose (4 140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	48	-0.005	-0.078	12.481	0.346	40	102	60	82	41	88 original
12363	72 [919; D-Xylopyranose (4 19 Alanine (BP) (3TMS)]	63	-0.006	-0.003	14.614	0.355	41	101	38	104	64	75 duplicate
7585	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	58	-0.008	-0.055	14.522	0.348	42	100	53	89	60	87 original
14893	72 [919; D-Xylopyranose (4 42 Glutamic acid	60	-0.008	-0.010	31.731	0.314	43	99	43	99	124	132 duplicate
7545	72 [919; D-Xylopyranose (4 89 [775; Dopamine (4TMS)]	35	-0.008	0.155	14.601	0.277	44	98	11	131	63	140 original
11228	72 [919; D-Xylopyranose (4 10 Glycine	63	-0.009	0.029	21.178	0.339	45	97	33	109	105	103 duplicate
7548	72 [919; D-Xylopyranose (4 92 [680; Glycerol-2-phosphate (4TMS)]	53	-0.010	-0.024	10.952	0.363	46	96	49	93	27	62 original
7547	72 [919; D-Xylopyranose (4 91 [766; beta-D-Methylglucopyranoside (4TMS)]	63	-0.011	0.017	18.295	0.369	47	95	34	108	96	48 original
7537	72 [919; D-Xylopyranose (4 81 Tyrosine	63	-0.017	-0.022	36.177	0.376	48	94	45	97	134	40 original
7597	72 [919; D-Xylopyranose (4 141 Lanosta-8,24-dien-3-beta-ol	60	-0.018	-0.091	12.063	0.334	49	93	68	76	38	112 original
7531	72 [919; D-Xylopyranose (4 75 Lysine	63	-0.027	-0.099	41.834	0.361	50	92	68	74	138	64 original
16414	72 [919; D-Xylopyranose (4 [636; 4R-Acetaldo-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	63	-0.030	-0.068	18.686	0.368	51	91	55	87	93	51 duplicate
7553	72 [919; D-Xylopyranose (4 97 [756; beta-D-Methylglucopyranoside (4TMS)]	51	-0.035	-0.009	23.228	0.364	52	89	42	100	110	24 original
12723	72 [919; D-Xylopyranose (4 22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	51	-0.035	-0.077	10.924	0.345	53	90	58	84	28	89 duplicate
11869	72 [919; D-Xylopyranose (4 15 Alanine	63	-0.036	-0.081	20.973	0.336	54	88	62	80	102	107 duplicate
7533	72 [919; D-Xylopyranose (4 [826; beta-[[[5-methyl-2-thienyl)methyl]eneamino-benzeneacetic acid methyl ester]	62	-0.039	-0.033	31.794	0.373	55	87	50	92	125	42 original
14284	72 [919; D-Xylopyranose (4 36 [598; N-Acetylglutamic acid (2TMS)]	63	-0.046	-0.089	30.889	0.338	56	86	65	77	122	104 duplicate
7559	72 [919; D-Xylopyranose (4 103 [948; Ethylamine (2TMS)]	62	-0.050	-0.060	17.453	0.352	57	85	54	88	88	79 original
7593	72 [919; D-Xylopyranose (4 137 Ergosterol	63	-0.055	-0.193	17.419	0.331	58	84	99	43	67	116 original
7589	72 [919; D-Xylopyranose (4 133 [855; Squalene]	63	-0.056	-0.134	11.019	0.357	59	82	74	68	29	71 original
16736	72 [919; D-Xylopyranose (4 82 [812; D-Xylofuranose (4TMS)]	63	-0.056	-0.173	16.662	0.327	60	83	91	51	82	124 duplicate
7561	72 [919; D-Xylopyranose (4 105 [705; 2-Ketogluconic acid (5TMS)]	47	-0.056	-0.072	14.745	0.377	61	81	56	86	68	38 original
14073	72 [919; D-Xylopyranose (4 34 Aspartic acid	63	-0.059	-0.023	34.949	0.338	62	80	48	84	133	105 duplicate
16003	72 [919; D-Xylopyranose (4 54 [NA]	54	-0.059	-0.248	13.200	0.351	63	79	116	26	45	80 duplicate
13639	72 [919; D-Xylopyranose (4 30 [815; Ethyl-3(2H)-thiophenone]	63	-0.061	0.002	32.065	0.358	64	77	37	105	127	70 duplicate
16498	72 [919; D-Xylopyranose (4 59 Ornithine; Arginine	63	-0.061	-0.045	43.015	0.353	65	78	52	90	139	78 duplicate
7552	72 [919; D-Xylopyranose (4 96 myo-Inositol	49	-0.061	-0.073	15.945	0.313	66	76	57	85	77	135 original
17332	72 [919; D-Xylopyranose (4 70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	-0.061	-0.148	21.158	0.336	67	75	79	63	104	108 duplicate
13189	72 [919; D-Xylopyranose (4 26 Citramalic acid	63	-0.062	-0.095	18.543	0.372	68	74	67	75	92	43 duplicate
13966	72 [919; D-Xylopyranose (4 33 Methionine	63	-0.065	0.005	12.721	0.338	69	73	36	106	43	106 duplicate
12841	72 [919; D-Xylopyranose (4 23 Homoserine	63	-0.068	0.047	12.629	0.343	70	72	28	114	42	95 duplicate
15739	72 [919; D-Xylopyranose (4 51 [498; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.070	0.006	16.625	0.294	71	71	35	107	81	138 duplicate
16577	72 [919; D-Xylopyranose (4 60 Glycerol-3-phosphate	63	-0.071	-0.118	23.772	0.340	72	70	71	71	112	101 duplicate
16331	72 [919; D-Xylopyranose (4 57 [757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	57	-0.072	-0.139	17.591	0.355	73	69	75	67	90	74 duplicate
10291	72 [919; D-Xylopyranose (4 3 Ethanolamine	62	-0.076	-0.079	10.899	0.343	74	68	61	81	25	99 duplicate
7581	72 [919; D-Xylopyranose (4 125 [692; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	63	-0.077	-0.082	34.116	0.345	75	67	64	78	130	90 original
10153	72 [919; D-Xylopyranose (4 2 Serine	62	-0.080	-0.174	21.900	0.358	76	66	92	50	108	68 duplicate
7549	72 [919; D-Xylopyranose (4 93 [507; Putrescine (4TMS)]	59	-0.080	-0.145	14.590	0.345	77	65	77	65	62	91 original
7544	72 [919; D-Xylopyranose (4 88 Gluconic acid	63	-0.081	-0.158	15.575	0.393	78	64	85	57	74	19 original
16967	72 [919; D-Xylopyranose (4 65 [646; 3-Deoxyglucitol (5TMS)]	62	-0.082	-0.183	16.943	0.379	79	63	95	47	85	34 duplicate
11616	72 [919; D-Xylopyranose (4 13 Uracil	63	-0.082	-0.146	19.306	0.368	80	62	78	64	97	49 duplicate
12118	72 [919; D-Xylopyranose (4 17 [700; 2-methyl-1,2-propanediol (2TMS)]	63	-0.083	-0.184	20.549	0.325	81	61	96	46	100	126 duplicate
17042	72 [919; D-Xylopyranose (4 66 Glyceric acid-3-phosphate	63	-0.086	-0.111	8.304	0.343	82	60	69	73	6	97 duplicate
12604	72 [919; D-Xylopyranose (4 21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	63	-0.085	-0.142	19.004	0.324	83	59	76	66	95	127 duplicate

15279	72 [919; D-Xylopyranose (4 46	Arabinose	63 -0,097	-0,156	21,143	0,341	84	57	82	60	103	100 duplicate	
16657	72 [919; D-Xylopyranose (4 61	[NA]	63 -0,097	-0,238	9,495	0,314	85	58	113	29	14	134 duplicate	
7584	72 [919; D-Xylopyranose (4 128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	44 -0,099	-0,290	11,804	0,361	86	56	132	10	35	63 original	
17189	72 [919; D-Xylopyranose (4 68	[570; Hypoxanthine (2TMS)]	19 -0,099	-0,020	12,283	0,312	87	55	44	98	37	138 duplicate	
7594	72 [919; D-Xylopyranose (4 136	[674; Ergosterol (1TMS)]	45 -0,111	-0,189	13,443	0,327	88	54	98	44	51	125 original	
11098	72 [919; D-Xylopyranose (4 9	Proline	62 -0,114	-0,160	30,440	0,376	89	52	86	56	121	39 duplicate	
16891	72 [919; D-Xylopyranose (4 64	[789; Tyramine (3TMS)]	62 -0,114	-0,317	8,483	0,345	90	53	134	8	9	92 duplicate	
7578	72 [919; D-Xylopyranose (4 123	[945; Galactofuranose-6-phosphate (7TMS)]	63 -0,114	-0,195	13,749	0,380	91	51	101	41	57	29 original	
11994	72 [919; D-Xylopyranose (4 16	[644; 2-Methyl-1,3-butanediol (2TMS)]	63 -0,120	-0,197	20,567	0,335	93	49	103	39	101	110 duplicate	
13749	72 [919; D-Xylopyranose (4 31	[822; Parabanic acid (2TMS)]	63 -0,121	-0,181	10,284	0,328	94	48	94	48	19	123 duplicate	
16247	72 [919; D-Xylopyranose (4 56	[829; Orolic acid (3TMS)]	63 -0,123	-0,153	14,136	0,360	95	46	80	62	58	65 duplicate	
12958	72 [919; D-Xylopyranose (4 24	[725; 2-Ketooctanoic acid (2TMS)]	63 -0,123	-0,180	34,362	0,346	96	47	83	49	131	86 duplicate	
17116	72 [919; D-Xylopyranose (4 67	Clitic acid	63 -0,124	-0,155	25,938	0,353	97	45	81	61	117	77 duplicate	
7580	72 [919; D-Xylopyranose (4 124	[734; 1-Monooctylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	58 -0,125	-0,124	20,292	0,393	98	44	72	70	99	20 original	
14593	72 [919; D-Xylopyranose (4 39	[829; 1-Phenylethanol (1TMS)]	62 -0,126	-0,221	20,118	0,317	99	43	109	33	98	130 duplicate	
7573	72 [919; D-Xylopyranose (4 117	[724; Glycerol (3TMS)]	55 -0,127	-0,167	11,520	0,398	100	42	90	52	34	16 original	
12241	72 [919; D-Xylopyranose (4 18	[590; 1-Acetyl-2-thiohydantoin]	63 -0,127	-0,194	10,961	0,346	101	41	100	42	28	85 duplicate	
11359	72 [919; D-Xylopyranose (4 11	Succinic acid	63 -0,130	-0,239	11,085	0,368	102	40	114	28	30	50 duplicate	
7560	72 [919; D-Xylopyranose (4 104	[785; Erythritol (4TMS)]	62 -0,130	-0,197	11,235	0,391	103	39	102	40	31	21 original	
7590	72 [919; D-Xylopyranose (4 134	Isomaltose	63 -0,133	-0,160	28,085	0,329	104	38	87	55	119	119 original	
7535	72 [919; D-Xylopyranose (4 79	Glucose	63 -0,136	-0,164	37,203	0,344	105	37	89	53	137	94 original	
7568	72 [919; D-Xylopyranose (4 110	[715; Erythritol (4TMS)]	53 -0,141	-0,222	13,306	0,408	106	36	59	83	47	13 original	
7577	72 [919; D-Xylopyranose (4 121	[657; Erythritol (4TMS)]	54 -0,145	-0,078	12,355	0,438	107	35	110	32	38	4 original	
14388	72 [919; D-Xylopyranose (4 37	Phenylalanine	63 -0,146	-0,187	25,012	0,382	108	34	97	45	114	25 duplicate	
7542	72 [919; D-Xylopyranose (4 86	[793; D-Galactono-1,4-lactone (4TMS)]	60 -0,147	-0,157	25,305	0,329	109	33	83	59	115	120 original	
7570	72 [919; D-Xylopyranose (4 114	Fructose-6-phosphate	52 -0,148	-0,269	10,374	0,459	110	32	126	16	22	2 original	
7568	72 [919; D-Xylopyranose (4 112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	7541	62 -0,149	-0,280	13,564	0,379	111	31	128	14	54	33 original
7565	72 [919; D-Xylopyranose (4 85	[529; Methylcitric acid (4TMS)]	48 -0,149	-0,287	7,835	0,380	112	30	129	13	5	31 original	
7550	72 [919; D-Xylopyranose (4 94	Octadecanoic acid	63 -0,150	-0,294	25,900	0,378	113	29	133	9	116	35 original	
11743	72 [919; D-Xylopyranose (4 14	Hexadecanoic acid	63 -0,151	-0,262	24,596	0,388	114	28	122	20	113	52 original	
7530	72 [919; D-Xylopyranose (4 74	Fumaric acid	63 -0,152	-0,204	9,161	0,333	115	27	105	37	12	115 duplicate	
10699	72 [919; D-Xylopyranose (4 6	Glycolic acid	63 -0,157	-0,220	13,365	0,408	116	26	108	34	49	12 original	
14491	72 [919; D-Xylopyranose (4 38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	63 -0,162	-0,163	43,728	0,382	117	25	88	54	141	26 duplicate	
7592	72 [919; D-Xylopyranose (4 106	[733; Threitol (4TMS)]	63 -0,163	-0,231	11,332	0,345	118	24	112	30	32	93 duplicate	
7592	72 [919; D-Xylopyranose (4 136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	61 -0,164	-0,223	14,975	0,374	119	23	111	31	71	41 original	
10966	72 [919; D-Xylopyranose (4 8	Isoleucine	17 -0,176	-0,260	5,803	0,333	120	22	121	21	1	114 original	
7567	72 [919; D-Xylopyranose (4 111	[583; Erythritol (4TMS)]	55 -0,177	-0,241	21,866	0,334	121	21	115	27	107	113 duplicate	
13528	72 [919; D-Xylopyranose (4 29	Erythritol	41 -0,178	-0,459	15,362	0,421	122	20	138	4	73	10 original	
7578	72 [919; D-Xylopyranose (4 122	[644; Erythritol (4TMS)]	63 -0,179	-0,257	8,851	0,370	123	19	119	23	10	47 duplicate	
7534	72 [919; D-Xylopyranose (4 78	Mannose	51 -0,181	-0,157	14,765	0,380	124	18	84	58	69	28 original	
11488	72 [919; D-Xylopyranose (4 12	Glyceric acid	61 -0,186	-0,211	13,543	0,358	125	17	106	36	53	69 original	
17402	72 [919; D-Xylopyranose (4 71	[731; Erythrose (3TMS)]	62 -0,187	-0,275	10,545	0,371	126	16	127	15	23	46 duplicate	
7591	72 [919; D-Xylopyranose (4 135		63 -0,191	-0,288	14,730	0,368	127	15	131	11	67	22 duplicate	
7569	72 [919; D-Xylopyranose (4 902;	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	63 -0,194	-0,288	14,675	0,365	128	14	130	12	65	57 original	
7571	72 [919; D-Xylopyranose (4 113	Galactose-6-phosphate	61 -0,209	-0,267	11,423	0,433	129	13	124	18	33	6 original	
10633	72 [919; D-Xylopyranose (4 115	Glucose-6-phosphate	61 -0,215	-0,253	27,557	0,390	130	12	117	25	118	30 original	
13416	72 [919; D-Xylopyranose (4 7	Threonine	63 -0,218	-0,263	32,425	0,367	131	11	123	19	128	53 duplicate	
7539	72 [919; D-Xylopyranose (4 28	Malic acid	63 -0,222	-0,269	12,373	0,364	132	10	125	17	39	60 duplicate	
			57 -0,226	-0,133	23,246	0,363	133	9	73	69	111	61 original	

7582	72 [918; D-Xylopyranose (4 126 [559; Erythritol (4TMS)]	44	-0.237	-0.351	10.341	0.431	134	8	136	6	21	7 original
7529	72 [919; D-Xylopyranose (4 73 [708; Glucose methoxyamine (5TMS)]	57	-0.249	-0.352	13.724	0.364	135	7	137	5	56	59 original
14179	72 [919; D-Xylopyranose (4 35 Pyrogulamic acid	63	-0.251	-0.255	43.365	0.356	136	6	118	24	140	72 duplicate
14694	72 [919; D-Xylopyranose (4 40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	63	-0.253	-0.336	36.493	0.365	137	5	135	7	135	65 duplicate
7556	72 [919; D-Xylopyranose (4 100 [657; Mannitol (6TMS)]	63	-0.260	-0.468	12.464	0.377	138	4	139	3	40	37 original
7532	72 [919; D-Xylopyranose (4 76 Fructose	63	-0.277	-0.215	28.416	0.379	139	3	107	35	120	32 original
7558	72 [919; D-Xylopyranose (4 102 [904; Galactose methoxyamine (5TMS)]	63	-0.288	-0.531	9.283	0.408	140	2	141	1	13	14 original
15086	72 [919; D-Xylopyranose (4 44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	49	-0.338	-0.499	14.562	0.434	141	1	140	2	61	5 duplicate
7610	73 [708; Glucose methoxy 86 [793; D-Galactono-1,4-lactone (4TMS)]	55	0.721	0.865	15.808	0.564	1	141	2	140	73	9 original
7600	73 [708; Glucose methoxy 76 Fructose	57	0.699	0.865	23.433	0.578	2	140	3	139	112	3 original
7630	73 [708; Glucose methoxy 106 [733; Threitol (4TMS)]	55	0.678	0.883	7.531	0.577	3	139	1	141	14	4 original
14180	73 [708; Glucose methoxy 35 Pyrogulamic acid	57	0.652	0.851	40.643	0.557	4	138	4	138	138	10 duplicate
7645	73 [708; Glucose methoxy 121 [657; Erythritol (4TMS)]	48	0.651	0.834	9.518	0.538	5	137	7	135	28	24 original
7602	73 [708; Glucose methoxy 78 Mannose	56	0.649	0.801	6.288	0.541	6	136	14	128	7	19 original
16248	73 [708; Glucose methoxy 56 [829; Orotic acid (3TMS)]	57	0.629	0.811	6.309	0.552	7	135	9	133	8	13 duplicate
16968	73 [708; Glucose methoxy 65 [646; 3-Deoxyglucitol (5TMS)]	57	0.622	0.803	8.033	0.540	8	134	13	129	16	22 duplicate
15280	73 [708; Glucose methoxy 46 Arabinose	57	0.618	0.805	12.816	0.541	9	133	11	131	54	20 duplicate
14695	73 [708; Glucose methoxy 115 Glucose-6-phosphate	55	0.617	0.840	23.866	0.506	10	132	5	137	114	47 original
11985	73 [708; Glucose methoxy 40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	57	0.617	0.839	35.039	0.567	11	130	6	136	134	8 duplicate
12959	73 [708; Glucose methoxy 16 [644; 2-Methyl-1,3-butanediol (2TMS)]	57	0.617	0.768	17.451	0.555	12	131	26	116	83	12 duplicate
14492	73 [708; Glucose methoxy 38 [708; 2-Ketogluconic acid (2TMS)]	57	0.614	0.786	30.645	0.556	13	128	19	123	123	11 duplicate
14594	73 [708; Glucose methoxy 39 [829; 1-Phenylethanol (1TMS)]	57	0.614	0.775	8.956	0.489	14	129	23	119	22	61 duplicate
7628	73 [708; Glucose methoxy 104 [795; Erythritol (4TMS)]	58	0.610	0.774	12.611	0.490	15	127	24	118	51	59 duplicate
7637	73 [708; Glucose methoxy 113 Galactose-6-phosphate	58	0.606	0.803	7.087	0.570	16	126	12	130	10	6 original
16737	73 [708; Glucose methoxy 62 [812; D-Xylofuranose (4TMS)]	55	0.605	0.815	5.609	0.537	17	125	8	134	3	25 original
7638	73 [708; Glucose methoxy 114 Fructose-6-phosphate	57	0.603	0.796	15.289	0.495	18	124	15	127	68	56 duplicate
13529	73 [708; Glucose methoxy 29 Erythritol	46	0.586	0.785	6.062	0.524	19	123	20	122	5	34 original
7634	73 [708; Glucose methoxy 110 [715; Erythritol (4TMS)]	57	0.584	0.757	8.266	0.502	20	122	27	115	20	50 duplicate
11617	73 [708; Glucose methoxy 13 Uracil	47	0.582	0.807	7.669	0.542	21	121	10	132	15	17 original
7641	73 [708; Glucose methoxy 117 [724; Glycerol (3TMS)]	57	0.575	0.753	14.849	0.569	22	120	29	113	64	7 duplicate
7646	73 [708; Glucose methoxy 122 [644; Erythritol (4TMS)]	49	0.573	0.790	5.394	0.473	23	119	16	126	2	69 original
7658	73 [708; Glucose methoxy 134 Isomaltose	45	0.572	0.787	11.827	0.520	24	118	17	125	43	38 original
12119	73 [708; Glucose methoxy 17 [700; 2-methyl-1,2-propanediol (2TMS)]	57	0.568	0.764	21.599	0.546	25	117	21	121	105	15 original
7649	73 [708; Glucose methoxy 125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	57	0.566	0.740	16.761	0.486	26	116	32	110	81	63 duplicate
13417	73 [708; Glucose methoxy 28 Malic acid	57	0.565	0.781	29.976	0.506	27	115	22	120	121	48 original
	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	57	0.559	0.769	11.232	0.507	28	114	25	117	41	46 duplicate
7653	73 [708; Glucose methoxy 11 Succinic acid	52	0.557	0.744	7.521	0.519	29	113	30	112	13	39 original
11360	73 [708; Glucose methoxy 50 [746; Ribonic acid-1,4-lactone (3TMS)]	57	0.549	0.754	9.723	0.473	30	112	28	114	30	70 duplicate
15650	73 [708; Glucose methoxy 44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	54	0.543	0.698	14.978	0.476	31	111	40	102	65	68 duplicate
15089	73 [708; Glucose methoxy 26 Citramalic acid	43	0.542	0.786	6.269	0.535	32	110	18	124	6	27 duplicate
16332	73 [708; Glucose methoxy 19 Alanine (BP) (3TMS)	48	0.539	0.725	9.471	0.488	33	109	35	107	27	62 duplicate
12364	73 [708; Glucose methoxy 22 [690; N,N-Di-(2-hydroxyethyl)-methanamine (2TMS)]	57	0.533	0.743	12.522	0.482	34	108	31	111	50	66 duplicate
12724	73 [708; Glucose methoxy 88 Gluconic acid	45	0.531	0.699	9.136	0.438	35	107	39	103	24	92 duplicate
7612	73 [708; Glucose methoxy 6 Glycerol	57	0.526	0.687	10.518	0.528	36	106	43	99	36	32 original
10700	73 [708; Glucose methoxy 14 Fumaric acid	57	0.521	0.736	41.493	0.515	37	103	33	109	140	42 duplicate
11744	73 [708; Glucose methoxy 123 [945; Galactofuranose-6-phosphate (7TMS)]	57	0.521	0.736	8.107	0.458	38	104	34	108	17	80 duplicate
7647	73 [708; Glucose methoxy 70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	0.521	0.712	12.748	0.521	39	105	38	104	53	37 original
17333	73 [708; Glucose methoxy 26 Citramalic acid	54	0.497	0.720	19.798	0.493	40	102	36	106	99	58 duplicate
13190	73 [708; Glucose methoxy 26 Citramalic acid	57	0.472	0.693	18.362	0.459	41	101	41	101	91	78 duplicate



12605	73 [708; Glucose methoxys 21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	57	0.465	0.638	17.676	0.465	42	100	48	94	85	75 duplicate
7607	73 [708; Glucose methoxys 83	Sorbitol	54	0.459	0.094	23.854	0.416	43	98	84	58	113	104 original
7650	73 [708; Glucose methoxys 126	[559; Erythritol (4TMS)]	38	0.457	0.179	6.021	0.543	44	98	37	105	4	16 original
7626	73 [708; Glucose methoxys 102	[904; Galactose methoxymine (5TMS)]	57	0.430	0.624	8.214	0.405	45	97	50	92	19	114 original
7624	73 [708; Glucose methoxys 100	[857; Mannitol (6TMS)]	57	0.424	0.623	11.174	0.423	46	95	51	91	40	101 original
14785	73 [708; Glucose methoxys 41	[639; Proline (2TMS)]	57	0.424	0.589	15.396	0.416	47	96	55	87	69	105 duplicate
7603	73 [708; Glucose methoxys 79	Glucose	57	0.416	0.692	34.621	0.503	48	94	42	100	132	49 original
7627	73 [708; Glucose methoxys 103	[648; Ethylamine (2TMS)]	56	0.416	0.477	12.701	0.463	49	93	65	77	52	76 original
16004	73 [708; Glucose methoxys 54	[NA]	48	0.402	0.665	9.535	0.440	50	92	45	97	29	80 duplicate
11489	73 [708; Glucose methoxys 12	Glycine acid	56	0.397	0.630	9.453	0.424	51	91	49	93	26	100 duplicate
7611	73 [708; Glucose methoxys 87	[945; beta-D-Glucopyranose (5TMS)]	55	0.380	0.677	32.797	0.456	53	89	44	98	129	83 original
7656	73 [708; Glucose methoxys 132	[895; Isomaltose methoxymine (8TMS)]	35	0.371	0.651	12.960	0.393	54	88	47	95	56	122 original
12242	73 [708; Glucose methoxys 18	[590; 1-Acetyl-2-thiohydantoin]	57	0.368	0.574	10.370	0.406	55	87	56	86	32	113 duplicate
7636	73 [708; Glucose methoxys 112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	56	0.338	0.549	13.690	0.399	56	86	57	85	58	120 original
7609	73 [708; Glucose methoxys 85	[529; Methylcitric acid (4TMS)]	48	0.337	0.595	8.532	0.456	57	85	53	89	21	84 original
7616	73 [708; Glucose methoxys 92	[680; Glycerol-2-phosphate (4TMS)]	47	0.332	0.594	7.514	0.434	58	84	54	88	12	95 original
7625	73 [708; Glucose methoxys 101	[832; Dopamine (4TMS)]	57	0.330	0.343	11.755	0.493	59	83	68	74	42	57 original
16892	73 [708; Glucose methoxys 64	[789; Tyramine (3TMS)]	56	0.322	0.453	9.076	0.400	60	82	66	76	23	119 duplicate
7644	73 [708; Glucose methoxys 120	[945; Uridine (3TMS)]	47	0.319	0.223	12.485	0.456	61	81	77	65	49	82 original
11870	73 [708; Glucose methoxys 15	Alanine	57	0.302	0.482	19.611	0.542	62	80	63	79	98	18 duplicate
135													
7659	73 [708; Glucose methoxys 902;	Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	57	0.301	0.483	15.085	0.382	63	79	64	78	67	129 original
7598	73 [708; Glucose methoxys 74	[912; Tetradecanoic acid (1TMS)]	57	0.288	0.653	8.179	0.531	64	77	46	96	18	30 original
7657	73 [708; Glucose methoxys 133	[855; Squalene]	57	0.286	0.391	10.481	0.376	65	78	67	75	35	132 original
7604	73 [708; Glucose methoxys 80	[772; D-Glucose (5TMS)]	55	0.282	0.545	30.187	0.422	66	76	58	84	122	103 original
7620	73 [708; Glucose methoxys 96	myo-Inositol	45	0.259	0.213	15.783	0.318	67	75	79	63	72	140 original
7623	73 [708; Glucose methoxys 99	[662; Ribose-5-phosphate methoxymine (9P) (5TMS)]	34	0.258	0.540	8.858	0.423	68	74	59	83	31	102 original
7615	73 [708; Glucose methoxys 91	[766; beta-D-Methylglucopyranoside (4TMS)]	57	0.252	0.224	16.513	0.462	69	73	76	68	78	78 original
7652	73 [708; Glucose methoxys 128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	38	0.223	0.492	7.160	0.410	70	72	62	80	11	109 original
7651	73 [708; Glucose methoxys 127	[777; Fructose-6-phosphate methoxymine (6TMS)]	32	0.218	0.295	6.649	0.391	71	71	72	70	9	124 original
7629	73 [708; Glucose methoxys 105	[705; 2-Ketoglucuronic acid (5TMS)]	41	0.210	0.222	10.890	0.472	72	70	78	64	38	72 original
7621	73 [708; Glucose methoxys 97	[756; beta-D-Methylglucopyranoside (4TMS)]	45	0.198	0.286	17.638	0.425	73	69	74	88	84	99 original
7640	73 [708; Glucose methoxys 116	[882; Pseudouridine (5TMS)]	30	0.182	0.322	9.337	0.386	74	68	69	73	25	127 original
7635	73 [708; Glucose methoxys 111	[583; Erythritol (4TMS)]	37	0.159	0.321	18.065	0.346	75	67	70	72	90	136 original
7633	73 [708; Glucose methoxys 108	Octadecanoic acid	57	0.157	0.622	22.464	0.525	76	65	52	90	109	33 original
17403	73 [708; Glucose methoxys 71	[731; Erythrose (3TMS)]	57	0.157	0.229	15.528	0.388	77	66	75	67	70	128 duplicate
7618	73 [708; Glucose methoxys 94	Hexadecanoic acid	57	0.100	0.498	22.963	0.513	78	64	61	81	111	43 original
7662	73 [708; Glucose methoxys 138	[674; Ergosterol (1TMS)]	42	0.099	0.291	13.671	0.426	79	63	73	69	57	97 original
16415													
7642	73 [708; Glucose methoxys 58	(1TMS)]	57	0.081	0.105	19.347	0.404	80	62	83	59	95	115 duplicate
7664	73 [708; Glucose methoxys 118	[928; Glucopyranose-6-phosphate (6TMS)]	51	0.038	0.170	10.473	0.365	81	61	80	62	34	133 original
7665	73 [708; Glucose methoxys 140	[892; Ergosta-7,22-dien-3-ol (1TMS)]	46	0.034	0.138	13.971	0.348	82	60	81	61	62	135 original
7654	73 [708; Glucose methoxys 130	Trehalose	55	0.028	0.128	12.334	0.412	83	59	82	60	47	107 original
7660	73 [708; Glucose methoxys 136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	56	0.022	-0.058	31.393	0.344	84	58	87	55	125	137 original
7661	73 [708; Glucose methoxys 137	Ergosterol	16	-0.017	0.313	3.852	0.472	85	57	71	71	1	71 original
7599	73 [708; Glucose methoxys 75	Lysine	57	-0.025	0.023	17.800	0.429	86	56	85	57	88	96 original
14285	73 [708; Glucose methoxys 35	[596; N-Acetylglutamic acid (2TMS)]	57	-0.040	-0.021	41.325	0.408	87	55	86	58	139	110 original
124													
7648	73 [708; Glucose methoxys 124	[734; 1-Monoleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]	57	-0.049	-0.130	31.528	0.396	88	54	91	51	127	121 duplicate
10834	73 [708; Glucose methoxys 7	Threonine	53	-0.078	-0.221	19.608	0.407	89	53	98	44	97	112 original
			57	-0.086	-0.112	32.148	0.407	90	52	80	52	128	111 duplicate

17043	73 [708; Glucose methoxyla	66	Glyceric acid-3-phosphate	57	-0.109	-0.160	10.727	0.411	91	51	93	49	37	108 duplicate
7663	73 [708; Glucose methoxyla	139	[700; Ergosta-5,7-dien-3-ol]	35	-0.119	-0.190	16.761	0.305	92	50	94	48	80	141 original
7617	73 [708; Glucose methoxyla	93	[607; Putrescine (4TMS)]	53	-0.132	-0.136	15.988	0.414	93	49	92	50	75	106 original
10015	73 [708; Glucose methoxyla	1	[938; Sulfuric acid (2TMS)]	29	-0.138	-0.090	10.380	0.453	94	48	88	54	33	85 duplicate
10429	73 [708; Glucose methoxyla	4	Phosphoric acid	50	-0.138	-0.276	36.061	0.342	95	47	102	40	136	138 duplicate
15374	73 [708; Glucose methoxyla	47	[NA]	67	-0.139	-0.205	15.062	0.401	96	46	96	46	66	118 duplicate
17190	73 [708; Glucose methoxyla	68	[570; Hypoxanthine (2TMS)]	17	-0.147	-0.865	11.064	0.530	97	45	139	3	39	31 duplicate
10154	73 [708; Glucose methoxyla	2	Serine	56	-0.168	-0.200	22.665	0.467	98	44	95	47	110	73 duplicate
7622	73 [708; Glucose methoxyla	98	[697; Ribose-5-phosphate methoxylamine (5TMS)]	43	-0.169	-0.529	16.613	0.484	99	43	119	23	79	65 original
7608	73 [708; Glucose methoxyla	84	Mannitol	55	-0.189	-0.092	31.005	0.381	100	42	89	53	124	130 original
15917	73 [708; Glucose methoxyla	53	Glycerol-2-phosphate	57	-0.187	-0.256	11.828	0.333	101	41	99	43	44	139 duplicate
13304	73 [708; Glucose methoxyla	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	49	-0.197	-0.594	20.113	0.497	102	40	122	20	100	55 duplicate
16578	73 [708; Glucose methoxyla	60	Glycerol-3-phosphate	57	-0.209	-0.271	24.664	0.384	103	39	101	41	117	128 duplicate
7614	73 [708; Glucose methoxyla	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	57	-0.216	-0.282	12.818	0.437	104	38	103	39	55	93 original
14992	73 [708; Glucose methoxyla	43	[548; Leucine (2TBS)]	53	-0.218	-0.421	13.800	0.403	105	37	114	28	60	67 duplicate
17117	73 [708; Glucose methoxyla	67	Citric acid	57	-0.224	-0.294	26.266	0.481	106	36	105	37	119	116 duplicate
7643	73 [708; Glucose methoxyla	119	[931; myo-Inositol-2-phosphate (7TMS)]	57	-0.231	-0.259	13.846	0.462	107	35	100	42	61	77 original
7631	73 [708; Glucose methoxyla	107	9-(Z)-Octadecenoic acid	57	-0.242	-0.350	18.396	0.392	108	34	109	33	92	123 original
12842	73 [708; Glucose methoxyla	23	Homoserine	57	-0.246	-0.595	17.708	0.507	109	33	123	19	86	45 duplicate
13750	73 [708; Glucose methoxyla	31	[622; Parabanic acid (2TMS)]	57	-0.249	-0.343	12.416	0.435	110	31	108	34	48	84 duplicate
17472	73 [708; Glucose methoxyla	72	[919; D-Xylopyranose (4TMS)]	57	-0.249	-0.352	13.724	0.364	111	32	110	32	59	134 duplicate
11099	73 [708; Glucose methoxyla	9	Proline	56	-0.262	-0.220	31.416	0.490	112	30	97	45	126	60 duplicate
7632	73 [708; Glucose methoxyla	108	Octadecenoic acid	57	-0.268	-0.370	11.892	0.388	113	29	112	30	45	125 original
14389	73 [708; Glucose methoxyla	37	Phenylalanine	57	-0.278	-0.365	25.622	0.402	114	28	111	31	118	117 duplicate
10987	73 [708; Glucose methoxyla	8	Isoleucine	51	-0.316	-0.268	21.707	0.450	115	27	104	38	106	86 duplicate
16815	73 [708; Glucose methoxyla	63	Glutamine	45	-0.321	-0.704	21.845	0.522	116	26	129	13	107	36 duplicate
14074	73 [708; Glucose methoxyla	34	Aspartic acid	57	-0.325	-0.333	35.336	0.441	117	25	107	35	135	89 duplicate
16658	73 [708; Glucose methoxyla	61	[NA]	57	-0.361	-0.452	12.331	0.426	118	24	115	27	46	98 duplicate
15829	73 [708; Glucose methoxyla	52	[NA]	39	-0.374	-0.699	20.368	0.498	119	23	128	14	102	53 duplicate
10292	73 [708; Glucose methoxyla	3	Ethanolamine	56	-0.388	-0.572	14.190	0.534	120	22	120	22	63	28 duplicate
13967	73 [708; Glucose methoxyla	33	Methionine	57	-0.400	-0.467	16.914	0.439	121	21	116	28	82	91 duplicate
13075	73 [708; Glucose methoxyla	25	[709; 2,5-Diaminovalerolactam (2TMS)]	41	-0.402	-0.620	17.758	0.518	122	20	125	17	87	40 duplicate
16497	73 [708; Glucose methoxyla	59	Ornithine; Arginine	57	-0.405	-0.316	42.691	0.456	123	19	106	36	141	81 duplicate
13859	73 [708; Glucose methoxyla	32	[729; N,N-Dimethyllysine methyl ester]	57	-0.409	-0.519	18.668	0.498	124	18	117	25	83	52 duplicate
13840	73 [708; Glucose methoxyla	30	[815; Ethyl-3(2H)-thiophenone]	57	-0.435	-0.391	33.488	0.448	125	17	113	29	130	88 duplicate
15185	73 [708; Glucose methoxyla	45	Homocysteine	54	-0.444	-0.632	18.990	0.449	126	16	126	16	94	87 duplicate
		77	[826; beta-[[[5-methyl-2-thienyl)methyl]ureaamino-benzeneacetic acid methyl ester]	56	-0.456	-0.526	34.471	0.497	127	15	118	24	131	54 original
7601	73 [708; Glucose methoxyla		benzeneacetic acid methyl ester]	43	-0.468	-0.660	18.016	0.485	128	14	127	15	89	64 duplicate
15740	73 [708; Glucose methoxyla	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	57	-0.479	-0.737	19.398	0.533	129	13	131	11	86	29 duplicate
15467	73 [708; Glucose methoxyla	48	Asparagine	57	-0.485	-0.578	38.008	0.586	130	12	121	21	137	2 original
7805	73 [708; Glucose methoxyla	81	Tyrosine	37	-0.485	-0.854	20.898	0.518	131	11	138	4	104	41 original
7613	73 [708; Glucose methoxyla	89	[775; Dopamine (4TMS)]	54	-0.522	-0.758	24.636	0.537	132	10	132	10	116	23 duplicate
11230	73 [708; Glucose methoxyla	10	Glycine	57	-0.530	-0.766	16.463	0.539	133	9	135	7	77	26 original
7619	73 [708; Glucose methoxyla	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	45	-0.541	-0.763	15.929	0.499	134	8	133	9	74	51 original
7655	73 [708; Glucose methoxyla	131	[626; 5-Methylthioadenosine (3TMS)]	49	-0.544	-0.838	20.652	0.540	135	7	137	5	103	21 duplicate
16090	73 [708; Glucose methoxyla	55	[612; 4-Aminobutyric acid (2TBS)]	42	-0.568	-0.763	27.204	0.551	136	6	134	8	120	14 duplicate
17262	73 [708; Glucose methoxyla	69	Arginine	54	-0.572	-0.727	21.952	0.512	137	5	130	12	108	44 duplicate
15559	73 [708; Glucose methoxyla	49	[877; Pyrophosphoric acid (4TMS)]	57	-0.580	-0.727	21.952	0.512	137	5	130	12	108	44 duplicate
14894	73 [708; Glucose methoxyla	42	Glutamic acid	54	-0.627	-0.607	34.766	0.466	138	4	124	18	133	74 duplicate
10565	73 [708; Glucose methoxyla	5	Leucine	45	-0.636	-0.808	16.363	0.524	139	3	136	6	76	35 duplicate

12485	73 [708; Glucose methoxys	20 [619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS))	31 -0.639	-0.914	15.623	0.574	140	2	140	2	71	5 duplicate
7606	73 [708; Glucose methoxys	82 Lysine	39 -0.646	-0.946	24.401	0.617	141	1	141	1	115	1 original
7676	74 [912; Tetradecanoic acid	85 [529; Methylcitric acid (4TMS))	48 0.637	0.854	7.785	0.579	1	141	4	138	7	4 original
7717	74 [912; Tetradecanoic acid	126 [559; Erythritol (4TMS))	45 0.616	0.857	5.483	0.517	2	140	3	139	1	27 original
15090	74 [912; Tetradecanoic acid	44 [910; 2-Ketogluconic acid methoxymethylamine (4TMS))	50 0.602	0.777	6.875	0.492	3	139	8	134	4	53 duplicate
7700	74 [912; Tetradecanoic acid	109 Octadecanoic acid	64 0.588	0.901	19.585	0.553	4	138	1	141	91	11 original
7723	74 [912; Tetradecanoic acid	132 [895; Isomaltose methoxymethylamine (8TMS))	42 0.577	0.713	13.090	0.421	5	137	16	126	48	101 original
7713	74 [912; Tetradecanoic acid	122 [644; Erythritol (4TMS))	52 0.575	0.790	11.706	0.522	6	136	6	136	41	24 original
7707	74 [912; Tetradecanoic acid	106 [882; Pseudouridine (5TMS))	30 0.563	0.629	8.292	0.372	7	135	30	112	11	130 original
7691	74 [912; Tetradecanoic acid	110 [857; Mannitol (6TMS))	64 0.557	0.687	10.284	0.467	8	134	22	120	27	69 original
14696	74 [912; Tetradecanoic acid	40 [680; 2,3-Dimethylsuccinic acid (2TMS))	64 0.554	0.777	35.554	0.574	9	133	7	135	134	5 duplicate
13418	74 [912; Tetradecanoic acid	28 Malic acid	64 0.540	0.767	10.579	0.496	10	132	10	132	28	40 duplicate
7701	74 [912; Tetradecanoic acid	110 [715; Erythritol (4TMS))	54 0.537	0.744	8.321	0.545	11	131	11	131	12	14 original
7693	74 [912; Tetradecanoic acid	102 [904; Galactose methoxymethylamine (5TMS))	64 0.533	0.674	7.982	0.460	12	130	23	119	8	79 original
7706	74 [912; Tetradecanoic acid	115 Glucose-6-phosphate	62 0.533	0.640	24.724	0.454	13	129	29	113	117	87 original
7708	74 [912; Tetradecanoic acid	117 [724; Glycerol (3TMS))	56 0.529	0.809	5.571	0.498	14	128	5	137	2	38 original
7685	74 [912; Tetradecanoic acid	94 Hexadecanoic acid	64 0.520	0.873	20.535	0.589	15	127	2	140	98	3 original
7705	74 [912; Tetradecanoic acid	114 Fructose-6-phosphate	53 0.517	0.697	7.719	0.475	16	126	21	121	6	62 original
7712	74 [912; Tetradecanoic acid	121 [657; Erythritol (4TMS))	55 0.516	0.770	11.247	0.485	17	125	9	133	35	50 original
7731	74 [912; Tetradecanoic acid	140 [692; Ergosta-7,22-dien-3-ol (1TMS))	49 0.515	0.615	14.989	0.461	18	124	34	108	63	76 original
7667	74 [912; Tetradecanoic acid	76 Fructose	64 0.510	0.622	25.093	0.509	19	123	32	110	118	29 original
7697	74 [912; Tetradecanoic acid	106 [733; Threitol (4TMS))	62 0.502	0.718	8.808	0.549	20	122	15	127	17	12 original
7729	74 [912; Tetradecanoic acid	138 [674; Ergosterol (1TMS))	46 0.498	0.741	14.981	0.496	21	121	13	129	62	42 original
11745	74 [912; Tetradecanoic acid	14 Fumaric acid	64 0.484	0.706	8.622	0.485	22	120	18	124	15	51 duplicate
7724	74 [912; Tetradecanoic acid	133 [855; Squalene]	64 0.477	0.537	8.853	0.513	23	119	49	93	18	28 original
14181	74 [912; Tetradecanoic acid	35 Pyroglutamic acid	64 0.468	0.591	42.034	0.470	24	118	38	104	139	68 duplicate
12725	74 [912; Tetradecanoic acid	22 [690; N,N-Di(2-Hydroxyethyl)-methanamine (2TMS))	52 0.468	0.711	9.791	0.530	25	117	17	125	24	21 duplicate
12606	74 [912; Tetradecanoic acid	21 [678; N,N-Di(2-Hydroxyethyl)-methanamine (2TMS))	64 0.465	0.668	17.424	0.481	26	116	25	117	78	54 duplicate
7703	74 [912; Tetradecanoic acid	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS))	63 0.461	0.704	15.189	0.501	27	115	19	123	65	38 original
12243	74 [912; Tetradecanoic acid	18 [590; 1-Acetyl-2-thiohydantoin]	64 0.461	0.697	9.261	0.487	28	114	20	122	20	46 duplicate
13191	74 [912; Tetradecanoic acid	26 Citramalic acid	64 0.454	0.743	17.847	0.472	29	113	12	130	81	67 duplicate
7732	74 [912; Tetradecanoic acid	141 Lanosta-8,24-dien-3-beta-ol	61 0.451	0.602	11.688	0.486	30	112	38	106	40	47 original
7726	74 [912; Tetradecanoic acid	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS))	64 0.448	0.740	14.123	0.475	31	111	14	128	56	63 original
7669	74 [912; Tetradecanoic acid	78 Mannose	62 0.435	0.674	8.335	0.558	32	110	24	118	13	9 original
7711	74 [912; Tetradecanoic acid	120 [945; Uridine (3TMS))	54 0.434	0.285	13.489	0.486	33	109	75	67	52	48 original
7704	74 [912; Tetradecanoic acid	113 Galactose-6-phosphate	62 0.421	0.579	8.240	0.424	34	108	41	101	10	99 original
11490	74 [912; Tetradecanoic acid	12 Glycercic acid	63 0.391	0.614	10.119	0.472	35	107	35	107	25	66 duplicate
7728	74 [912; Tetradecanoic acid	137 Ergosterol	64 0.389	0.446	14.637	0.412	36	106	61	81	61	106 original
16738	74 [912; Tetradecanoic acid	62 [812; D-Xylofuranose (4TMS))	64 0.384	0.584	15.383	0.450	37	104	40	102	68	88 duplicate
7716	74 [912; Tetradecanoic acid	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64 0.384	0.455	32.249	0.412	38	105	60	82	128	105 original
12365	74 [912; Tetradecanoic acid	19 Alanine (BP) (3TMS)	64 0.360	0.641	12.192	0.496	40	102	28	114	43	41 duplicate
11361	74 [912; Tetradecanoic acid	11 Succinic acid	64 0.353	0.576	9.789	0.465	41	101	42	100	23	70 duplicate
7677	74 [912; Tetradecanoic acid	86 [793; D-Galactono-1,4-lactone (4TMS))	61 0.353	0.594	19.983	0.504	42	100	37	105	95	32 original
14493	74 [912; Tetradecanoic acid	38 [708; 2,3-Dimethylsuccinic acid (2TMS))	64 0.348	0.649	9.055	0.499	43	99	27	115	19	37 duplicate
14796	74 [912; Tetradecanoic acid	111 [639; Proline (2TMS))	64 0.323	0.617	14.453	0.503	44	98	33	109	60	34 duplicate
7702	74 [912; Tetradecanoic acid	111 [583; Erythritol (4TMS))	42 0.322	0.515	19.934	0.405	45	97	56	88	93	111 original
15651	74 [912; Tetradecanoic acid	50 [746; Ribonic acid-1,4-lactone (3TMS))	61 0.314	0.529	16.608	0.533	46	96	54	88	73	18 duplicate
14595	74 [912; Tetradecanoic acid	39 [829; 1-Phenylethanol (1TMS))	63 0.310	0.624	15.073	0.494	47	95	31	111	64	52 duplicate
17334	74 [912; Tetradecanoic acid	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS))	57 0.306	0.375	19.637	0.400	48	94	64	78	82	113 duplicate

7695	74 [912]; Tetradecanoic acid	104	[795; Erythritol (4TMS)]	63	0.295	0.535	8.639	0.503	49	83	52	90	16	35 original
17541	74 [912]; Tetradecanoic acid	73	[708; Glucose methoxyamine (5TMS)]	57	0.286	0.653	8.179	0.531	50	92	28	116	9	19 duplicate
13530	74 [912]; Tetradecanoic acid	29	Erythritol	64	0.285	0.549	8.544	0.526	51	90	47	95	14	22 duplicate
7714	74 [912]; Tetradecanoic acid	123	[945; Galactofuranose-6-phosphate (7TMS)]	64	0.285	0.528	12.370	0.474	52	91	55	87	46	64 original
16249	74 [912]; Tetradecanoic acid	56	[829; Orlic acid (3TMS)]	64	0.271	0.537	10.235	0.478	53	89	50	92	26	60 duplicate
12960	74 [912]; Tetradecanoic acid	24	[725; 2-Ketooctanoic acid (2TMS)]	64	0.268	0.563	32.507	0.520	54	88	44	98	128	26 duplicate
11618	74 [912]; Tetradecanoic acid	13	Uracil	64	0.266	0.550	16.467	0.560	55	87	46	96	72	8 duplicate
16005	74 [912]; Tetradecanoic acid	54	[NA]	55	0.262	0.437	11.594	0.391	56	86	62	80	38	122 duplicate
7679	74 [912]; Tetradecanoic acid	88	Gluconic acid	64	0.261	0.532	12.224	0.544	57	85	53	89	44	15 original
7674	74 [912]; Tetradecanoic acid	83	Sorbitol	58	0.257	0.163	22.397	0.384	58	84	81	61	109	125 original
15281	74 [912]; Tetradecanoic acid	46	Arabinose	64	0.255	0.536	16.694	0.473	59	83	51	91	74	65 duplicate
16969	74 [912]; Tetradecanoic acid	65	[646; 3-Deoxyglucitol (5TMS)]	63	0.253	0.585	11.646	0.461	60	82	39	103	39	74 duplicate
11996	74 [912]; Tetradecanoic acid	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	0.252	0.546	18.491	0.555	61	81	48	94	85	10 duplicate
16333	74 [912]; Tetradecanoic acid	57	[757; 2-Desoxy-pentos-3-yose dimethoxyamine (2TMS)]	55	0.251	0.511	13.140	0.433	62	80	57	85	49	95 duplicate
7725	74 [912]; Tetradecanoic acid	134	Isomaltose	64	0.248	0.565	24.562	0.490	63	79	43	99	115	45 original
7720	74 [912]; Tetradecanoic acid	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	0.246	0.554	10.656	0.480	64	78	45	97	30	55 original
7687	74 [912]; Tetradecanoic acid	86	myo-Inositol	49	0.243	0.306	18.620	0.321	65	77	73	69	88	138 original
10701	74 [912]; Tetradecanoic acid	6	Glycerol	64	0.225	0.336	42.855	0.461	66	76	68	74	141	75 duplicate
17404	74 [912]; Tetradecanoic acid	71	[731; Erythrose (3TMS)]	64	0.224	0.424	14.217	0.477	67	75	63	79	58	59 duplicate
7730	74 [912]; Tetradecanoic acid	139	[700; Ergosta-5,7-dien-3-ol]	38	0.223	0.220	18.864	0.297	68	74	78	64	89	140 original
7710	74 [912]; Tetradecanoic acid	119	[931; myo-Inositol-2-phosphate (7TMS)]	64	0.207	0.307	10.580	0.445	69	73	72	70	29	93 original
12120	74 [912]; Tetradecanoic acid	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	0.201	0.478	18.319	0.454	70	72	59	83	84	86 duplicate
7719	74 [912]; Tetradecanoic acid	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.192	0.347	9.484	0.317	71	71	67	75	21	139 original
7715	74 [912]; Tetradecanoic acid	124	[734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	59	0.191	0.169	22.036	0.405	72	70	80	62	105	110 original
7683	74 [912]; Tetradecanoic acid	92	[680; Glycerol-2-phosphate (4TMS)]	54	0.182	0.283	10.768	0.358	73	69	74	68	31	135 original
7718	74 [912]; Tetradecanoic acid	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.163	0.366	7.701	0.294	74	68	65	77	5	141 original
7698	74 [912]; Tetradecanoic acid	107	9-Z-Octadecenoic acid	64	0.150	0.124	16.800	0.371	75	67	84	58	76	132 original
7678	74 [912]; Tetradecanoic acid	87	[945; beta-D-Glucopyranose (5TMS)]	62	0.134	0.361	35.700	0.388	76	66	68	76	135	123 original
7694	74 [912]; Tetradecanoic acid	103	[648; Ethylamine (2TMS)]	63	0.127	0.259	15.805	0.455	77	65	76	66	88	85 original
7727	74 [912]; Tetradecanoic acid	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.118	0.332	6.506	0.329	78	64	69	73	3	137 original
7681	74 [912]; Tetradecanoic acid	90	[910; 9-Z-Hexadecenoic acid (1TMS)]	64	0.114	0.073	11.190	0.393	79	63	87	55	34	121 original
7670	74 [912]; Tetradecanoic acid	79	Glucose	64	0.110	0.313	35.854	0.422	80	62	71	71	136	100 original
7675	74 [912]; Tetradecanoic acid	84	Mannitol	62	0.099	-0.067	33.888	0.415	81	61	95	47	131	103 original
16893	74 [912]; Tetradecanoic acid	64	[789; Tyramine (3TMS)]	63	0.058	0.135	9.703	0.353	82	60	83	59	22	136 duplicate
7671	74 [912]; Tetradecanoic acid	80	[772; D-Glucose (5TMS)]	62	0.053	0.247	31.757	0.384	83	59	77	65	124	124 original
7696	74 [912]; Tetradecanoic acid	105	[705; 2-Ketogluconic acid (5TMS)]	48	0.051	0.212	13.495	0.463	84	58	79	63	53	72 original
7709	74 [912]; Tetradecanoic acid	118	[928; Glucopyranose-6-phosphate (6TMS)]	58	0.020	0.119	11.505	0.373	85	57	85	57	37	129 original
7692	74 [912]; Tetradecanoic acid	101	[832; Dopamine (4TMS)]	64	0.020	0.063	14.245	0.397	86	55	88	54	59	116 original
7682	74 [912]; Tetradecanoic acid	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	0.020	-0.023	20.413	0.456	87	56	93	49	96	83 original
12486	74 [912]; Tetradecanoic acid	20	[619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	31	0.019	-0.579	15.862	0.614	88	54	128	14	69	1 duplicate
16579	74 [912]; Tetradecanoic acid	60	Glycerol-3-phosphate	64	0.019	0.143	23.144	0.427	89	53	82	60	112	98 duplicate
11871	74 [912]; Tetradecanoic acid	15	Alanine	64	0.014	0.092	20.465	0.431	90	52	86	56	97	96 duplicate
17118	74 [912]; Tetradecanoic acid	67	Citric acid	64	0.011	0.057	25.534	0.399	91	51	89	53	119	114 duplicate
15918	74 [912]; Tetradecanoic acid	53	Glycerol-2-phosphate	64	-0.015	-0.317	12.714	0.444	92	50	114	28	47	94 duplicate
7688	74 [912]; Tetradecanoic acid	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	-0.017	0.044	22.616	0.399	93	49	90	52	110	115 original
7690	74 [912]; Tetradecanoic acid	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	-0.039	0.328	11.780	0.487	94	48	70	72	42	39 original
7721	74 [912]; Tetradecanoic acid	130	Trehalose	63	-0.040	-0.075	31.540	0.368	95	47	88	46	123	133 original

14288	74 [912]; Tetradecanoic acid	36	[596; N-Acetylglutamic acid (2TMS)]	64	-0,050	-0,022	30,391	0,394	96	46	92	50	122	119 duplicate
7699	74 [912]; Tetradecanoic acid	108	Octadecanoic acid	64	-0,058	-0,081	11,155	0,376	97	45	97	45	33	128 original
7684	74 [912]; Tetradecanoic acid	93	[607; Putrescine (4TMS)]	60	-0,060	-0,178	17,638	0,397	98	44	103	39	79	117 original
10835	74 [912]; Tetradecanoic acid	7	Threonine	64	-0,077	-0,008	31,769	0,394	99	43	91	51	125	118 duplicate
14390	74 [912]; Tetradecanoic acid	37	Phenylalanine	64	-0,115	-0,097	24,719	0,427	100	42	99	43	116	97 duplicate
15375	74 [912]; Tetradecanoic acid	47	[NA]	64	-0,134	-0,286	16,035	0,491	101	41	110	32	70	44 duplicate
16416	74 [912]; Tetradecanoic acid	58	[636; 4R-Acetaldo-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	-0,153	-0,035	18,724	0,371	102	40	94	48	88	131 duplicate
17473	74 [912]; Tetradecanoic acid	72	[918; D-Xylopyranose (4TMS)]	63	-0,157	-0,220	13,365	0,408	103	39	107	35	51	108 duplicate
10016	74 [912]; Tetradecanoic acid	1	[938; Sulfuric acid (2TMS)]	82	-0,168	-0,216	12,284	0,459	104	38	106	36	45	80 duplicate
10293	74 [912]; Tetradecanoic acid	3	Ethanolamine	82	-0,185	-0,276	13,765	0,449	105	37	109	33	54	91 duplicate
10430	74 [912]; Tetradecanoic acid	4	Phosphoric acid	51	-0,186	-0,122	34,460	0,363	106	36	100	42	132	134 duplicate
7666	74 [912]; Tetradecanoic acid	75	Lysine	64	-0,191	-0,088	41,207	0,405	107	35	98	44	138	112 original
15741	74 [912]; Tetradecanoic acid	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	64	-0,197	-0,453	18,710	0,520	108	34	123	19	87	25 duplicate
7672	74 [912]; Tetradecanoic acid	81	Tyrosine	64	-0,216	-0,265	36,362	0,545	109	33	108	34	137	13 original
16659	74 [912]; Tetradecanoic acid	61	[NA]	64	-0,231	-0,288	11,480	0,379	110	32	112	30	36	127 duplicate
17044	74 [912]; Tetradecanoic acid	66	Glycine acid-3-phosphate	64	-0,235	-0,191	10,885	0,457	111	31	104	38	32	82 duplicate
14895	74 [912]; Tetradecanoic acid	42	Glutamic acid	60	-0,252	-0,343	33,204	0,455	112	30	115	27	130	84 duplicate
15830	74 [912]; Tetradecanoic acid	52	[NA]	46	-0,258	-0,415	18,972	0,475	113	29	118	24	90	61 duplicate
16091	74 [912]; Tetradecanoic acid	55	[612; 4-Aminobutyric acid (2TBS)]	43	-0,262	-0,444	21,572	0,478	114	28	121	21	103	57 duplicate
7668	74 [912]; Tetradecanoic acid	77	[826; beta-[[[(5-methyl-2-thienyl)methyleneamino]-benzeneacetic acid methyl ester]	62	-0,264	-0,286	32,454	0,460	115	27	111	31	127	78 original
16498	74 [912]; Tetradecanoic acid	59	Omithine; Arginine	64	-0,275	-0,300	42,733	0,407	116	26	113	29	140	109 duplicate
10968	74 [912]; Tetradecanoic acid	8	Isoleucine	55	-0,300	-0,165	21,913	0,393	117	25	101	41	104	120 duplicate
11100	74 [912]; Tetradecanoic acid	9	Proline	63	-0,308	-0,204	30,388	0,410	118	24	105	37	121	107 duplicate
7686	74 [912]; Tetradecanoic acid	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	60	-0,309	-0,561	15,795	0,536	119	23	125	17	67	17 original
10155	74 [912]; Tetradecanoic acid	2	Serine	62	-0,324	-0,168	22,298	0,415	120	22	102	40	108	102 duplicate
13751	74 [912]; Tetradecanoic acid	31	[622; Parabanic acid (2TMS)]	64	-0,328	-0,428	13,809	0,447	121	21	120	22	55	92 duplicate
11231	74 [912]; Tetradecanoic acid	10	Glycine	64	-0,340	-0,607	23,301	0,485	122	20	129	13	113	49 duplicate
13641	74 [912]; Tetradecanoic acid	30	[815; Ethyl-3-(2H)-thiophenone]	64	-0,348	-0,371	32,773	0,449	123	19	116	26	129	90 duplicate
15468	74 [912]; Tetradecanoic acid	48	Asparagine	64	-0,358	-0,579	18,236	0,480	124	18	127	15	82	56 duplicate
17263	74 [912]; Tetradecanoic acid	69	Arginine	60	-0,366	-0,570	25,811	0,523	125	17	126	16	120	23 duplicate
13968	74 [912]; Tetradecanoic acid	33	Methionine	64	-0,370	-0,451	16,693	0,495	126	16	122	20	75	43 duplicate
7722	74 [912]; Tetradecanoic acid	131	[626; 5-Methylthioadenosine (3TMS)]	55	-0,374	-0,743	17,317	0,536	127	15	139	3	77	16 original
13860	74 [912]; Tetradecanoic acid	32	[728; N,N-Dimethyllysine methyl ester]	63	-0,386	-0,407	19,951	0,567	128	14	117	25	94	7 duplicate
10566	74 [912]; Tetradecanoic acid	5	Leucine	45	-0,390	-0,757	18,423	0,589	129	13	140	2	71	2 duplicate
14075	74 [912]; Tetradecanoic acid	34	Aspartic acid	64	-0,395	-0,418	35,256	0,460	130	12	119	23	133	77 duplicate
7673	74 [912]; Tetradecanoic acid	82	Lysine	39	-0,401	-0,802	22,088	0,570	131	11	141	1	108	6 original
7689	74 [912]; Tetradecanoic acid	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	48	-0,411	-0,674	18,307	0,530	132	10	136	6	83	20 original
15186	74 [912]; Tetradecanoic acid	45	Homocysteine	61	-0,412	-0,628	21,181	0,461	133	9	130	12	102	73 duplicate
12843	74 [912]; Tetradecanoic acid	23	Homoserine	64	-0,415	-0,666	17,703	0,507	134	8	135	7	80	30 duplicate
13305	74 [912]; Tetradecanoic acid	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	-0,422	-0,657	22,155	0,505	135	7	133	9	107	31 duplicate
17191	74 [912]; Tetradecanoic acid	68	[570; Hypoxanthine (2TMS)]	20	-0,453	-0,730	13,311	0,464	136	6	137	5	50	71 duplicate
16816	74 [912]; Tetradecanoic acid	63	Glutamine	52	-0,471	-0,515	20,489	0,413	137	5	124	18	98	104 duplicate
15560	74 [912]; Tetradecanoic acid	49	[877; Pyrophosphoric acid (4TMS)]	35	-0,480	-0,742	23,649	0,503	138	4	138	4	114	33 duplicate
7680	74 [912]; Tetradecanoic acid	89	[775; Dopamine (4TMS)]	60	-0,482	-0,657	20,826	0,478	139	3	132	10	101	58 original
14993	74 [912]; Tetradecanoic acid	43	[546; Leucine (2TBS)]	60	-0,489	-0,656	14,151	0,449	140	2	131	11	57	89 duplicate
13076	74 [912]; Tetradecanoic acid	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0,523	-0,660	20,671	0,459	141	1	134	8	100	81 duplicate
16417	75 Lysine	58	[636; 4R-Acetaldo-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	0,755	0,920	25,701	0,541	1	141	1	141	38	111 duplicate
10156	75 Lysine	2	Serine	62	0,570	0,875	28,104	0,552	2	140	3	139	46	6 duplicate

11101	75 Lysine	9	Proline	63	0.520	0.891	20,008	0.535	3	139	2	140	25	13 duplicate
17045	75 Lysine	66	Glyceric acid-3-phosphate	64	0.492	0.794	40,304	0.482	4	138	6	138	100	36 duplicate
13306	75 Lysine	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	0.485	0.889	47,294	0.471	5	137	14	128	126	37 duplicate
13861	75 Lysine	32	[729; N,N-Dimethyllysine methyl ester]	63	0.476	0.782	45,498	0.496	6	136	8	134	119	29 duplicate
7787	75 Lysine	130	Trehalose	63	0.467	0.578	10,444	0.406	7	135	25	117	8	85 original
16489	75 Lysine	59	Ornithine; Arginine	64	0.460	0.850	3,458	0.534	8	134	4	138	1	14 duplicate
14287	75 Lysine	36	[596; N-Acetylglutamic acid (2TMS)]	64	0.457	0.737	12,500	0.543	9	133	11	131	11	10 duplicate
13752	75 Lysine	31	[622; Parabanic acid (2TMS)]	64	0.437	0.854	44,827	0.434	10	132	18	124	117	64 duplicate
10838	75 Lysine	7	Threonine	64	0.432	0.837	10,060	0.519	11	131	5	137	7	19 duplicate
7755	75 Lysine	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	48	0.402	0.524	48,411	0.410	12	130	31	111	128	81 original
11232	75 Lysine	10	Glycine	64	0.393	0.555	23,459	0.455	13	129	28	114	31	46 duplicate
7738	75 Lysine	81	Tyrosine	64	0.392	0.673	10,840	0.543	14	128	17	125	9	9 original
10431	75 Lysine	4	Phosphoric acid	51	0.391	0.685	5,096	0.558	15	127	16	126	2	5 duplicate
12844	75 Lysine	23	Homoserine	64	0.372	0.571	36,153	0.441	16	126	26	116	75	57 duplicate
13969	75 Lysine	33	Methionine	64	0.365	0.609	36,316	0.444	17	125	21	121	78	54 duplicate
13642	75 Lysine	30	[815; Ethyl-3(2H)-thiophenone]	64	0.359	0.735	13,963	0.508	18	124	12	130	12	24 duplicate
10294	75 Lysine	62	Ethandiamine	62	0.352	0.590	44,354	0.496	19	123	23	119	114	28 duplicate
14896	75 Lysine	60	Glutamic acid	60	0.351	0.754	18,948	0.523	20	122	10	132	21	18 duplicate
10969	75 Lysine	8	Isoleucine	55	0.344	0.788	26,529	0.558	21	121	7	135	40	4 duplicate
16894	75 Lysine	64	[789; Tyramine (3TMS)]	63	0.334	0.285	38,771	0.356	22	120	41	101	90	117 duplicate
7736	75 Lysine	79	Glucose	64	0.317	0.100	10,961	0.493	23	119	53	89	10	31 original
11872	75 Lysine	15	Alanine	64	0.316	0.238	24,025	0.418	24	118	44	88	32	74 duplicate
7734	75 Lysine	77	[826; beta-[[[5-methyl-2-thienyl]methyl]amino- benzeneacetic acid methyl ester]	62	0.313	0.759	15,851	0.545	25	117	9	133	14	8 original
14076	75 Lysine	34	Aspartic acid	64	0.305	0.614	9,733	0.448	26	116	20	122	6	53 duplicate
14391	75 Lysine	37	Phenylalanine	64	0.267	0.688	17,616	0.525	27	115	15	127	18	16 duplicate
17264	75 Lysine	69	Arginine	60	0.267	0.582	23,312	0.515	28	114	24	118	30	21 duplicate
17192	75 Lysine	98	[570; Hypoxanthine (2TMS)]	20	0.263	0.454	33,323	0.369	29	113	32	110	62	106 duplicate
14894	75 Lysine	43	[548; Leucine (2TBS)]	60	0.232	0.200	34,762	0.375	30	112	48	94	68	102 duplicate
16580	75 Lysine	60	Glycerol-3-phosphate	64	0.228	0.592	19,223	0.503	31	111	22	120	22	25 duplicate
13077	75 Lysine	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	0.216	0.532	39,198	0.427	32	110	30	112	94	69 duplicate
7780	75 Lysine	123	[845; Galactoturanose-6-phosphate (7TMS)]	64	0.210	0.315	30,919	0.450	33	109	38	104	55	50 original
7795	75 Lysine	138	[674; Ergosterol (1TMS)]	46	0.208	0.337	45,125	0.360	34	108	36	106	118	115 original
7740	75 Lysine	83	Sorbitol	58	0.208	0.724	20,116	0.538	35	107	13	129	26	12 original
15469	75 Lysine	48	Asparagine	64	0.206	0.346	37,406	0.424	36	106	34	108	83	71 duplicate
17119	75 Lysine	67	Citric acid	64	0.194	0.629	16,615	0.422	37	105	19	123	18	72 duplicate
7761	75 Lysine	104	[795; Erythritol (4TMS)]	63	0.192	0.238	37,823	0.417	38	104	45	97	86	76 original
15742	75 Lysine	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	0.182	0.553	49,531	0.499	39	103	29	113	131	27 duplicate
15187	75 Lysine	45	Homocysteine	61	0.173	0.247	56,022	0.417	40	102	43	99	139	75 duplicate
7788	75 Lysine	131	[626; 5-Methylthiadenosine (3TMS)]	55	0.166	0.105	48,924	0.408	41	101	52	90	130	64 original
7790	75 Lysine	133	[855; Squalene]	64	0.163	0.362	36,891	0.382	42	100	33	109	81	88 original
7765	75 Lysine	108	Octadecanoic acid	64	0.132	0.301	40,938	0.354	43	99	40	102	102	119 original
7781	75 Lysine	124	[734; 1-Monoleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]	59	0.122	0.333	57,398	0.373	44	98	37	105	140	103 original
7771	75 Lysine	114	Fructose-6-phosphate	53	0.112	0.041	38,784	0.409	45	97	60	82	91	82 original
17405	75 Lysine	71	[731; Erythrose (3TMS)]	64	0.106	0.559	28,911	0.461	46	96	27	115	50	43 duplicate
16660	75 Lysine	61	[NA]	64	0.101	0.123	37,639	0.339	47	95	50	92	84	131 duplicate
7775	75 Lysine	118	[928; Glucopyranose-6-phosphate (6TMS)]	58	0.080	0.068	39,511	0.312	48	94	57	85	86	138 original
12368	75 Lysine	19	Alanine (BP) (3TMS)	64	0.081	0.058	31,027	0.366	49	93	58	84	56	93 duplicate
10567	75 Lysine	5	Leucine	45	0.081	0.338	38,215	0.551	50	92	35	107	89	7 duplicate
14797	75 Lysine	41	[639; Proline (2TMS)]	64	0.072	0.109	28,221	0.385	51	91	51	91	47	95 duplicate

7770	75 Lysine	113	Galactose-6-phosphate	62	0.068	-0.043	41.507	0.430	52	90	68	74	107	66 original
7768	75 Lysine	111	[583; Erythritol (4TMS)]	42	0.029	0.094	48.048	0.280	53	89	55	87	127	140 original
7764	75 Lysine	137	Ergosterol	64	0.011	0.279	30.280	0.362	54	88	42	100	54	113 original
7752	75 Lysine	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	0.006	0.190	50.286	0.355	55	87	49	93	132	118 original
15561	75 Lysine	49	[877; Pyrophosphoric acid (4TMS)]	64	0.005	-0.027	53.787	0.354	56	88	67	75	138	120 duplicate
7751	75 Lysine	94	Hexadecanoic acid	64	-0.007	0.215	21.581	0.365	57	85	47	95	28	111 original
7768	75 Lysine	109	Octadecanoic acid	64	-0.008	0.218	24.580	0.346	58	84	46	98	34	126 original
7763	75 Lysine	138	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.015	0.311	19.413	0.321	59	83	39	103	24	136 original
12487	75 Lysine	20	[619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.024	-0.142	39.655	0.528	60	82	76	66	97	15 duplicate
10702	75 Lysine	6	Glycerol	64	-0.026	-0.152	8.010	0.365	61	81	80	62	3	109 duplicate
17474	75 Lysine	72	[919; D-Xylopyranose (4TMS)]	63	-0.027	-0.099	41.834	0.361	62	80	74	68	108	114 duplicate
7766	75 Lysine	139	[700; Ergosta-5,7-dien-3-ol]	38	-0.033	0.071	44.631	0.285	63	79	56	86	116	139 original
7739	75 Lysine	82	Lysine	39	-0.036	0.049	24.452	0.571	64	78	59	83	33	2 original
17542	75 Lysine	73	[708; Glucose methoxyamine (5TMS)]	57	-0.040	-0.021	41.325	0.408	65	77	68	78	106	83 duplicate
17335	75 Lysine	96	myo-Inositol	49	-0.058	-0.101	51.146	0.394	66	76	75	67	134	98 original
7737	75 Lysine	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	-0.060	-0.016	22.869	0.411	67	75	65	77	29	80 duplicate
14182	75 Lysine	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	49	-0.065	-0.075	46.765	0.347	68	74	70	72	125	125 original
12244	75 Lysine	80	[772; D-Glucose (5TMS)]	62	-0.069	-0.210	17.684	0.338	69	73	85	57	19	133 original
7783	75 Lysine	35	Pyroglutamic acid	64	-0.080	-0.220	8.654	0.395	70	72	86	56	5	91 duplicate
7773	75 Lysine	126	[590; 1-Acetyl-2-thiohydantoin]	64	-0.083	-0.090	34.931	0.363	71	71	73	69	70	112 duplicate
7778	75 Lysine	116	[559; Erythritol (4TMS)]	45	-0.085	0.033	34.378	0.511	72	70	62	80	65	22 original
7776	75 Lysine	118	[882; Pseudouridine (5TMS)]	30	-0.090	-0.376	31.204	0.489	73	69	103	39	57	34 original
7733	75 Lysine	121	[657; Erythritol (4TMS)]	55	-0.096	-0.070	45.755	0.365	74	68	69	73	120	110 original
7798	75 Lysine	64	Fructose	64	-0.100	-0.245	21.581	0.367	75	67	88	54	27	107 original
15831	75 Lysine	61	-0.103	0.003	46.228	0.461	77	65	63	79	123	41	duplicate	
7772	75 Lysine	46	-0.107	-0.193	18.001	0.386	78	64	83	59	20	94	original	
7774	75 Lysine	115	Glucose-6-phosphate	62	-0.108	-0.147	37.816	0.420	79	63	77	65	85	73 original
7742	75 Lysine	85	[529; Methylcitric acid (4TMS)]	56	-0.109	-0.148	35.402	0.566	80	62	78	64	72	3 original
7763	75 Lysine	106	[733; Threitol (4TMS)]	62	-0.111	-0.187	35.855	0.489	81	61	84	58	74	35 original
7746	75 Lysine	89	[775; Dopamine (4TMS)]	35	-0.123	0.036	37.932	0.461	82	60	61	81	87	42 original
16092	75 Lysine	55	[612; 4-Aminobutyric acid (2TBS)]	43	-0.127	-0.298	52.361	0.584	83	59	98	46	136	1 duplicate
7735	75 Lysine	78	Mannose	62	-0.130	-0.271	43.121	0.342	84	58	90	52	109	128 original
15919	75 Lysine	53	Glycerol-2-phosphate	64	-0.141	-0.260	46.158	0.366	85	57	89	53	122	108 duplicate
7767	75 Lysine	110	[715; Erythritol (4TMS)]	54	-0.145	-0.176	40.491	0.523	86	56	82	60	101	17 original
14697	75 Lysine	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.154	-0.282	8.178	0.439	87	55	91	51	4	60 duplicate
7782	75 Lysine	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	-0.157	-0.242	16.668	0.378	88	54	87	55	17	101 original
7776	75 Lysine	119	[931; myo-Inositol-2-phosphate (7TMS)]	64	-0.161	-0.148	36.513	0.352	89	53	79	63	79	122 original
7764	75 Lysine	107	9-(Z)-Octadecenoic acid	64	-0.167	-0.002	26.821	0.340	90	52	64	78	42	130 original
15091	75 Lysine	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	-0.174	-0.157	32.343	0.448	91	51	81	61	59	51 duplicate
17609	75 Lysine	74	[912; Tetradecanoic acid (1TMS)]	62	-0.181	-0.088	41.207	0.405	93	49	72	70	105	87 duplicate
7744	75 Lysine	87	[945; beta-D-Glucopyranose (5TMS)]	62	-0.183	-0.282	16.259	0.370	94	48	92	50	15	104 original
16817	75 Lysine	63	Glutamine	52	-0.185	0.095	40.122	0.349	95	47	54	88	88	124 duplicate
13419	75 Lysine	28	Malic acid	64	-0.189	-0.460	32.940	0.425	96	46	109	33	61	70 duplicate
7779	75 Lysine	122	[644; Erythritol (4TMS)]	52	-0.217	-0.297	45.780	0.492	97	45	95	47	121	32 original
12607	75 Lysine	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	-0.218	-0.438	25.280	0.404	98	44	108	34	36	88 duplicate
13192	75 Lysine	26	Citramalic acid	64	-0.223	-0.359	24.679	0.363	99	43	101	41	35	97 duplicate
11746	75 Lysine	14	Fumaric acid	64	-0.245	-0.495	44.364	0.443	100	42	112	30	15	55 duplicate
7784	75 Lysine	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	39	-0.247	-0.361	28.855	0.250	101	41	102	40	48	141 original
7789	75 Lysine	132	[895; Isomaltose methoxyamine (8TMS)]	42	-0.250	-0.503	41.153	0.314	102	40	114	28	104	137 original

7748	75 Lysine	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	-0.251	-0.689	40.180	0.502	103	39	138	4	99	26 original
7758	75 Lysine	101	[832; Dopamine (4TMS)]	64	-0.255	-0.614	38.082	0.511	104	38	132	10	88	23 original
7777	75 Lysine	120	[945; Uridine (3TMS)]	54	-0.258	-0.339	26.836	0.369	105	37	100	42	43	105 original
7759	75 Lysine	102	[904; Galactose methoxyamine (5TMS)]	64	-0.258	-0.314	40.977	0.345	106	36	98	44	103	128 original
15376	75 Lysine	47	[NA]	64	-0.272	-0.480	39.331	0.431	107	35	111	31	95	65 duplicate
18739	75 Lysine	62	[812; D-Xylofuranose (4TMS)]	64	-0.280	-0.431	27.649	0.381	108	34	107	35	44	100 duplicate
7747	75 Lysine	90	[910; 9-(2)-Hexadecenoic acid (1TMS)]	64	-0.284	-0.286	36.160	0.338	109	32	93	49	76	132 original
7757	75 Lysine	100	[857; Mannitol (6TMS)]	64	-0.284	-0.421	33.824	0.357	110	33	108	36	63	116 original
7760	75 Lysine	103	[848; Ethylamine (2TMS)]	63	-0.292	-0.608	37.245	0.442	111	31	131	11	82	56 original
7743	75 Lysine	88	[793; D-Galactono-1,4-lactone (4TMS)]	61	-0.294	-0.420	34.017	0.454	112	30	105	37	64	47 original
12726	75 Lysine	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	-0.305	-0.559	43.944	0.451	113	29	122	20	113	49 duplicate
14494	75 Lysine	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.313	-0.571	35.741	0.413	114	28	125	17	73	79 duplicate
11362	75 Lysine	11	Succinic acid	64	-0.318	-0.500	35.075	0.403	115	27	113	29	71	89 duplicate
7769	75 Lysine	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	-0.320	-0.389	52.051	0.397	116	26	104	38	135	90 original
7792	75 Lysine	135		64	-0.324	-0.290	29.016	0.353	117	25	94	48	51	121 original
16250	75 Lysine	56	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	-0.325	-0.506	43.652	0.448	118	24	115	27	110	62 duplicate
14596	75 Lysine	99	[829; Orolic acid (3TMS)]	63	-0.335	-0.565	32.635	0.416	119	23	123	19	60	77 duplicate
7791	75 Lysine	34	[829; 1-Phenylethanol (1TMS)]	64	-0.336	-0.539	25.719	0.440	120	22	120	22	39	58 original
11619	75 Lysine	13	Uracil	64	-0.340	-0.601	28.869	0.468	121	21	128	14	49	38 duplicate
7745	75 Lysine	88	Gluconic acid	64	-0.353	-0.577	34.450	0.492	122	20	126	16	68	33 original
12121	75 Lysine	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	-0.355	-0.571	26.603	0.456	123	19	124	18	41	45 duplicate
11997	75 Lysine	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	-0.362	-0.620	25.466	0.468	124	18	134	8	37	39 duplicate
13531	75 Lysine	29	Erythritol	64	-0.371	-0.622	39.041	0.458	125	17	135	7	92	44 duplicate
12961	75 Lysine	24	[725; 2-Ketobutanolic acid (2TMS)]	64	-0.372	-0.591	14.802	0.466	126	16	127	15	13	40 duplicate
7786	75 Lysine	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	59	-0.373	-0.538	39.181	0.405	127	15	119	23	93	88 original
15652	75 Lysine	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	-0.384	-0.614	53.685	0.453	128	14	133	9	137	48 duplicate
16970	75 Lysine	65	[646; 3-Deoxyglucitol (5TMS)]	63	-0.390	-0.524	43.879	0.436	129	13	118	24	112	63 duplicate
7754	75 Lysine	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	-0.392	-0.647	27.820	0.495	130	12	137	5	45	30 original
15282	75 Lysine	46	Arabinose	64	-0.403	-0.521	34.801	0.440	131	11	117	25	69	59 duplicate
7749	75 Lysine	92	[880; Glycerol-2-phosphate (4TMS)]	54	-0.410	-0.330	36.697	0.352	132	10	99	43	80	123 original
11491	75 Lysine	12	Glyceric acid	63	-0.419	-0.605	46.304	0.390	133	9	130	12	124	92 duplicate
16334	75 Lysine	57	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55	-0.429	-0.461	34.462	0.427	134	8	110	32	67	68 duplicate
7785	75 Lysine	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	-0.448	-0.543	29.444	0.337	135	7	121	21	52	134 original
7756	75 Lysine	99	[682; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	-0.451	-0.628	36.221	0.345	136	6	136	6	77	127 original
16006	75 Lysine	83	[607; Putrescine (4TMS)]	60	-0.473	-0.511	50.431	0.416	137	5	116	26	133	78 original
10017	75 Lysine	54	[NA]	55	-0.500	-0.601	43.669	0.428	138	4	129	13	111	67 duplicate
7741	75 Lysine	1	[938; Sulfuric acid (2TMS)]	36	-0.537	-0.755	29.948	0.438	139	3	140	2	53	61 duplicate
7762	75 Lysine	62	[705; 2-Ketogluconic acid (5TMS)]	48	-0.574	-0.863	19.302	0.517	140	2	141	1	23	20 original
7828	76 Fructose	84	Mannitol	62	0.803	0.934	18.318	0.438	141	1	139	3	58	62 original
14698	76 Fructose	105	[705; 2-Ketogluconic acid (5TMS)]	62	0.803	0.934	18.318	0.438	141	1	139	3	58	62 original
15092	76 Fructose	108	[733; Threitol (4TMS)]	64	0.780	0.858	15.134	0.592	2	140	24	118	28	37 duplicate
7832	76 Fructose	40	[880; 2,3-Dimethylsuccinic acid (2TMS)]	50	0.783	0.912	21.312	0.666	3	139	12	130	60	12 duplicate
7844	76 Fructose	110	[715; Erythritol (4TMS)]	54	0.779	0.926	27.214	0.655	4	138	7	135	102	15 original
7839	76 Fructose	122	[644; Erythritol (4TMS)]	52	0.772	0.884	33.774	0.605	5	137	18	123	120	30 original
7843	76 Fructose	117	[724; Glycerol (3TMS)]	56	0.757	0.812	24.239	0.606	6	136	38	104	82	29 original
7837	76 Fructose	121	[657; Erythritol (4TMS)]	55	0.756	0.837	32.708	0.601	7	135	31	111	117	34 original
14183	76 Fructose	115	Glucose-6-phosphate	62	0.741	0.964	4.875	0.651	8	134	3	139	1	16 original
		35	Pyroglutamic acid	64	0.736	0.970	19.287	0.671	9	133	1	141	46	7 duplicate



7800	76 Fructose	78 Mannose	62	0.728	0.901	25.508	0.614	10	132	14	128	93	24 original
7848	76 Fructose	126 [559; Erythritol (4TMS)]	45	0.723	0.898	26.294	0.605	11	131	15	127	98	32 original
17543	76 Fructose	73 [708; Glucose methoxyamine (5TMS)]	57	0.699	0.865	23.433	0.578	12	130	22	120	77	47 duplicate
13420	76 Fructose	28 Malic acid	64	0.690	0.845	18.098	0.603	13	129	29	113	41	33 duplicate
7808	76 Fructose	86 [793; D-Galactono-1,4-lactone (4TMS)]	61	0.677	0.965	12.746	0.695	14	128	2	140	13	1 original
14495	76 Fructose	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.656	0.857	19.899	0.608	15	127	27	115	50	28 duplicate
11747	76 Fructose	14 Fumaric acid	64	0.633	0.830	28.738	0.568	16	128	34	108	107	65 duplicate
12892	76 Fructose	24 [725; 2-Ketotolanoic acid (2TMS)]	64	0.623	0.887	10.015	0.693	17	125	17	125	7	4 duplicate
16251	76 Fructose	56 [829; Orolic acid (3TMS)]	64	0.616	0.921	25.180	0.664	18	124	10	132	90	13 duplicate
16740	76 Fructose	62 [812; D-Xylofuranose (4TMS)]	64	0.614	0.894	13.223	0.599	19	123	16	126	18	35 duplicate
11898	76 Fructose	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	64	0.611	0.862	9.669	0.667	20	122	28	114	5	9 duplicate
15283	76 Fructose	48 Arabinose	64	0.610	0.935	14.262	0.669	21	121	5	137	23	8 duplicate
14597	76 Fructose	39 [829; 1-Phenylethanol (1TMS)]	63	0.605	0.857	13.947	0.616	22	120	26	116	22	23 duplicate
7856	76 Fructose	134 Isomaltose	64	0.601	0.917	6.307	0.681	23	119	11	131	2	5 original
12727	76 Fructose	22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.593	0.764	29.745	0.573	24	118	43	99	108	49 duplicate
13532	76 Fructose	29 Erythritol	64	0.592	0.808	23.897	0.562	25	117	41	101	81	58 duplicate
16971	76 Fructose	65 [646; 3-Deoxyglucitol (5TMS)]	63	0.591	0.922	25.029	0.666	26	116	9	133	87	11 duplicate
11363	76 Fructose	11 Succinic acid	64	0.585	0.836	19.851	0.567	27	115	32	110	49	54 duplicate
17336	76 Fructose	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	0.584	0.754	8.768	0.549	28	114	44	98	4	82 duplicate
7822	76 Fructose	100 [857; Mannitol (6TMS)]	64	0.582	0.840	19.062	0.508	29	113	55	87	44	63 original
11620	76 Fructose	13 Uracil	64	0.581	0.858	11.182	0.687	30	112	25	117	9	10 duplicate
7847	76 Fructose	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru Glc]	64	0.574	0.940	8.093	0.619	31	111	4	138	3	21 original
7851	76 Fructose	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D- Glc]	59	0.565	0.880	22.759	0.648	32	110	20	122	67	17 original
7835	76 Fructose	113 Galactose-6-phosphate	62	0.562	0.923	25.460	0.574	33	109	8	134	92	48 original
7810	76 Fructose	88 Gluconic acid	64	0.559	0.831	16.666	0.643	34	108	33	109	35	18 original
12608	76 Fructose	21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	0.557	0.704	11.884	0.513	35	107	51	91	11	80 duplicate
12122	76 Fructose	17 [700; 2-methyl-1,2-propanediol (2TMS)]	64	0.553	0.844	9.854	0.560	36	106	30	112	6	59 duplicate
7824	76 Fructose	102 [804; Galactose methoxyamine (5TMS)]	64	0.547	0.605	26.069	0.528	37	105	60	82	96	74 original
7836	76 Fructose	114 Fructose-6-phosphate	53	0.536	0.886	25.610	0.534	38	104	18	124	94	46 original
13193	76 Fructose	26 Citramalic acid	64	0.530	0.735	12.808	0.534	39	103	47	95	14	72 duplicate
15653	76 Fructose	50 [746; Ribonic acid-1,4-lactone (3TMS)]	61	0.523	0.806	38.537	0.571	40	102	40	102	136	53 duplicate
10703	76 Fructose	6 Glyceral	64	0.511	0.859	20.352	0.592	42	100	23	119	55	40 duplicate
17810	76 Fructose	74 [912; Tetradecanoic acid (1TMS)]	64	0.510	0.822	25.093	0.509	43	99	57	85	88	82 duplicate
16335	76 Fructose	57 [757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55	0.502	0.907	19.444	0.632	44	98	13	128	47	20 duplicate
7826	76 Fructose	104 [795; Erythritol (4TMS)]	63	0.501	0.723	22.183	0.538	45	97	48	94	65	69 original
11492	76 Fructose	12 Glyceralic acid	63	0.494	0.712	30.983	0.535	46	96	50	92	112	70 duplicate
7854	76 Fructose	132 [895; Isomaltose methoxyamine (8TMS)]	42	0.477	0.791	31.304	0.591	47	95	42	100	113	41 original
7842	76 Fructose	120 [945; Uridine (3TMS)]	54	0.470	0.300	16.130	0.554	48	94	74	68	33	61 original
12367	76 Fructose	19 Alanine (BP) (3TMS)	64	0.469	0.814	15.482	0.546	49	93	37	105	29	64 duplicate
7834	76 Fructose	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.469	0.803	37.145	0.490	50	92	61	81	134	91 original
12245	76 Fructose	103 [648; Ethylamine (2TMS)]	64	0.465	0.608	20.446	0.449	51	91	59	83	56	108 duplicate
7825	76 Fructose	135	63	0.445	0.667	19.976	0.527	52	90	53	89	51	75 original
7857	76 Fructose	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	0.421	0.464	16.318	0.480	53	89	69	73	34	94 original
16007	76 Fructose	54 [NA]	55	0.417	0.820	28.924	0.568	54	88	36	108	110	56 duplicate
7807	76 Fructose	85 [529; Methyldictric acid (4TMS)]	48	0.401	0.590	19.529	0.488	55	87	63	79	48	92 original
7845	76 Fructose	123 [945; Galactofuranose-6-phosphate (7TMS)]	64	0.392	0.747	16.725	0.531	56	86	45	97	37	73 original
7814	76 Fructose	92 [680; Glycerol-2-phosphate (4TMS)]	54	0.378	0.875	23.689	0.595	57	85	21	121	80	36 original
14798	76 Fructose	41 [639; Proline (2TMS)]	64	0.371	0.635	14.414	0.494	58	84	56	88	25	89 duplicate

7823	76 Fructose	101 [832; Dopamine (4TMS)]	64 0.343	0.561	21.614	0.506	59	83	64	78	63	86 original
7801	76 Fructose	79 Glucose	64 0.340	0.810	13.003	0.572	60	82	39	103	17	51 original
7850	76 Fructose	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45 0.333	0.716	20.186	0.572	61	81	49	93	54	52 original
7809	76 Fructose	87 [945; beta-D-Glucopyranose (5TMS)]	62 0.333	0.824	12.933	0.538	62	80	35	107	16	68 original
7805	76 Fructose	83 Sorbitol	58 0.286	-0.084	14.897	0.330	63	79	86	56	27	141 original
7833	76 Fructose	111 [583; Erythritol (4TMS)]	42 0.287	0.368	38.879	0.452	64	78	71	137	104 original	
7813	76 Fructose	91 [766; beta-D-Methylglucopyranoside (4TMS)]	64 0.272	0.480	23.442	0.448	65	77	67	75	78	107 original
7818	76 Fructose	96 myo-Inositol	49 0.257	0.222	36.581	0.346	66	76	76	66	132	137 original
7827	76 Fructose	105 [705; 2-Ketogluconic acid (5TMS)]	48 0.252	0.486	21.542	0.582	67	75	66	76	61	45 original
7855	76 Fructose	133 [855; Squelene]	64 0.243	0.186	23.390	0.365	68	74	77	65	76	136 original
7819	76 Fructose	97 [756; beta-D-Methylglucopyranoside (4TMS)]	52 0.232	0.594	15.736	0.518	69	73	62	80	30	79 original
7831	76 Fructose	109 Octadecanoic acid	64 0.231	0.472	13.514	0.523	70	72	68	74	19	78 original
7802	76 Fructose	80 [772; D-Glucose (5TMS)]	62 0.224	0.746	10.345	0.510	71	71	46	96	8	81 original
16895	76 Fructose	64 [789; Tyramine (3TMS)]	63 0.211	0.488	24.881	0.421	72	70	65	77	85	118-tuplicate
11873	76 Fructose	15 Alanine	64 0.202	0.611	11.212	0.612	73	69	58	84	10	26-tuplicate
7849	76 Fructose	127 [777; Fructose-6-phosphate methoxamine (6TMS)]	39 0.190	0.438	22.903	0.609	74	68	70	72	70	27 original
7860	76 Fructose	138 [674; Ergosterol (1TMS)]	46 0.181	0.178	33.690	0.481	75	67	78	64	119	93 original
7816	76 Fructose	94 Hexadecanoic acid	64 0.181	0.343	12.268	0.499	76	66	72	70	12	87 original
7838	76 Fructose	116 [882; Pseudouridine (5TMS)]	30 0.177	0.233	20.719	0.508	77	65	75	67	59	85 original
7862	76 Fructose	140 [892; Ergosta-7,22-dien-3-ol (1TMS)]	49 0.170	0.119	33.194	0.469	78	64	81	61	118	88 original
7821	76 Fructose	99 [862; Ribose-5-phosphate methoxamine (BP) (5TMS)]	41 0.148	0.703	27.390	0.563	79	63	52	90	104	57 original
7863	76 Fructose	141 Lanosta-8,24-dien-3-beta-ol	61 0.090	-0.041	33.834	0.478	80	62	84	58	122	85 original
7406	76 Fructose	71 [731; Erythrose (3TMS)]	64 0.038	-0.078	17.164	0.417	81	61	85	57	39	123-tuplicate
7859	76 Fructose	137 Ergosterol	64 0.034	-0.133	20.144	0.442	82	60	88	54	53	109 original
7806	76 Fructose	84 Mannitol	62 0.006	0.143	16.860	0.402	83	59	80	62	38	126 original
7840	76 Fructose	118 [928; Glucopyranose-6-phosphate (6TMS)]	58 -0.014	0.338	27.071	0.449	84	58	73	69	100	105 original
7846	76 Fructose	124 [734; 1-Monoleoylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	59 -0.015	-0.289	43.611	0.418	85	57	97	45	140	122 original
15377	76 Fructose	47 [NA]	64 -0.051	0.057	25.438	0.448	86	56	82	60	91	108-tuplicate
6418	76 Fructose	[536; 4R-Acclamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64 -0.056	-0.149	17.379	0.330	87	55	90	52	40	140-tuplicate
7815	76 Fructose	93 [507; Putrescine (4TMS)]	60 -0.060	-0.009	36.526	0.427	88	54	83	59	131	116 original
7852	76 Fructose	130 Trehalose	63 -0.081	-0.147	13.760	0.367	89	53	89	53	21	134 original
7841	76 Fructose	119 [931; myo-Inositol-2-phosphate (7TMS)]	64 -0.084	-0.351	24.263	0.541	90	52	102	40	83	66 original
7876	76 Fructose	75 Lysine	64 -0.100	-0.245	21.581	0.367	91	51	95	47	62	133-tuplicate
7861	76 Fructose	139 [700; Ergosta-5,7-dien-3-ol]	38 -0.101	-0.216	34.334	0.398	92	50	93	49	124	127 original
7812	76 Fructose	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	64 -0.114	-0.289	23.319	0.418	93	49	96	46	75	121 original
4288	76 Fructose	36 [596; N-Acetylglutamic acid (2TMS)]	64 -0.123	-0.295	15.867	0.371	94	48	98	44	31	132-tuplicate
0432	76 Fructose	4 Phosphoric acid	51 -0.128	-0.200	18.265	0.339	95	47	91	51	42	138-tuplicate
5920	76 Fructose	53 Glycerol-2-phosphate	64 -0.130	-0.228	31.983	0.366	96	46	94	48	114	135-tuplicate
7858	76 Fructose	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17 -0.132	-0.126	16.099	0.463	97	45	87	55	32	100 original
7829	76 Fructose	107 9-(Z)-Octadecenoic acid	64 -0.156	-0.436	16.704	0.427	98	44	106	36	36	117 original
0837	76 Fructose	7 Threonine	64 -0.167	-0.314	14.777	0.380	99	43	99	43	26	129-tuplicate
7046	76 Fructose	66 Glyceral acid-3-phosphate	64 -0.207	-0.366	27.301	0.435	100	42	103	39	103	112-tuplicate
0157	76 Fructose	2 Serine	62 -0.222	-0.344	22.848	0.404	101	41	101	41	68	125-tuplicate
7120	76 Fructose	67 Citric acid	64 -0.251	-0.540	12.910	0.457	102	40	110	32	15	102-tuplicate
6581	76 Fructose	60 Glycerol-3-phosphate	36 -0.261	-0.492	14.398	0.467	103	39	107	35	24	99-tuplicate
0018	76 Fructose	1 [938; Sulfuric acid (2TMS)]	36 -0.263	0.158	24.446	0.559	104	38	79	63	84	60-tuplicate
7475	76 Fructose	72 [919; D-Xylopyranose (4TMS)]	63 -0.277	-0.215	28.416	0.379	105	37	92	50	108	130-tuplicate
3307	76 Fructose	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53 -0.298	-0.621	36.043	0.491	106	36	118	24	128	90-tuplicate
7830	76 Fructose	108 Octadecanoic acid	64 -0.300	-0.493	28.228	0.419	107	35	108	34	105	120 original

13753	76 Fructose	31	[622; Parabenic acid (2TMS)]	64	-0.305	-0.528	32.084	0.453	108	34	109	33	115	103 duplicate
11102	76 Fructose	8	Proline	63	-0.305	-0.413	23.271	0.379	109	33	105	37	74	131 duplicate
10970	76 Fructose	9	Isoleucine	55	-0.333	-0.334	20.632	0.339	110	32	100	42	57	139 duplicate
14392	76 Fructose	37	Phenylalanine	64	-0.335	-0.553	13.528	0.420	111	31	112	30	20	119 duplicate
14895	76 Fructose	43	[548; Leucine (2TBS)]	60	-0.360	-0.379	22.433	0.472	112	30	104	38	68	96 duplicate
12845	76 Fructose	52	Homoserine	64	-0.393	-0.701	27.081	0.525	113	29	123	19	101	76 duplicate
15832	76 Fructose	23	[NA]	46	-0.393	-0.846	38.767	0.592	114	28	133	9	133	39 duplicate
10295	76 Fructose	3	Ethanolamine	62	-0.402	-0.773	32.347	0.587	115	27	127	15	116	42 duplicate
17193	76 Fructose	68	[570; Hypoxanthine (2TMS)]	20	-0.411	-0.919	23.023	0.583	116	26	137	5	71	44 duplicate
7820	76 Fructose	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	48	-0.418	-0.663	35.965	0.540	117	25	121	21	127	67 original
16661	76 Fructose	61	[NA]	64	-0.434	-0.608	25.132	0.497	118	24	115	27	89	88 duplicate
13862	76 Fructose	32	[729; N,N-Dimethyllysine methyl ester]	63	-0.436	-0.631	35.782	0.534	119	23	119	23	128	71 duplicate
14077	76 Fructose	34	Aspartic acid	64	-0.450	-0.543	19.284	0.439	120	22	111	31	45	110 duplicate
16500	76 Fructose	59	Omithine; Arginine	64	-0.463	-0.569	23.641	0.439	121	21	113	29	79	111 duplicate
16818	76 Fructose	63	Glutamine	52	-0.472	-0.865	34.285	0.640	122	20	134	8	123	19 duplicate
7803	76 Fructose	81	Tyrosine	64	-0.484	-0.779	23.183	0.613	123	19	129	13	73	25 original
7799	76 Fructose	77	[826; beta-[(5-methyl-2-thienyl)methyl]neamino-benzeneacetic acid methyl ester]	62	-0.502	-0.671	23.126	0.427	124	18	122	20	72	115 original
13970	76 Fructose	33	Methionine	64	-0.505	-0.619	27.003	0.472	125	17	117	25	99	97 duplicate
15743	76 Fructose	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.507	-0.708	34.943	0.459	126	16	124	18	125	101 duplicate
13643	76 Fructose	30	[815; Ethyl-3(2H)-thiophenone]	64	-0.521	-0.587	20.694	0.382	127	15	114	28	58	128 duplicate
7817	76 Fructose	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	-0.527	-0.800	36.285	0.525	128	14	131	11	130	77 original
15470	76 Fructose	48	Asparagine	64	-0.531	-0.884	29.169	0.618	129	13	135	7	108	22 duplicate
11233	76 Fructose	10	Glycine	64	-0.545	-0.886	20.074	0.678	130	12	136	6	52	6 duplicate
15188	76 Fructose	45	Homocysteine	61	-0.550	-0.641	42.052	0.413	131	11	120	22	139	124 duplicate
14897	76 Fructose	42	Glutamic acid	60	-0.553	-0.774	33.783	0.548	133	9	128	14	121	114 duplicate
13078	76 Fructose	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.566	-0.782	21.929	0.573	134	8	130	12	64	50 duplicate
17265	76 Fructose	69	Arginine	60	-0.592	-0.930	37.747	0.592	135	7	138	4	135	38 duplicate
16093	76 Fructose	55	[612; 4-Aminobutyric acid (2TBS)]	43	-0.592	-0.830	26.053	0.542	136	6	125	17	95	65 duplicate
10568	76 Fructose	5	Leucine	45	-0.626	-0.817	36.218	0.605	137	5	132	10	129	31 original
7853	76 Fructose	131	[826; 5-Methylthioadenosine (3TMS)]	55	-0.630	-0.817	36.218	0.605	137	5	132	10	129	31 original
7811	76 Fructose	89	[775; Dopamine (4TMS)]	35	-0.637	-0.956	30.350	0.583	138	4	139	3	111	43 original
12488	76 Fructose	20	[619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.639	-0.972	26.267	0.655	139	3	141	1	97	14 duplicate
16562	76 Fructose	49	[877; Pyrophosphoric acid (4TMS)]	64	-0.663	-0.732	41.949	0.507	140	2	128	16	138	84 duplicate
7804	76 Fructose	82	Lysine	39	-0.760	-0.964	22.901	0.689	141	1	140	2	69	2 original
7867	76 Fructose	82	Lysine	62	0.847	0.933	7.560	0.591	1	141	1	141	3	8 original
7868	77 [826; beta-[(5-methyl-2-)]	81	Tyrosine	39	0.779	0.902	15.959	0.594	2	140	6	136	18	6 original
14898	77 [826; beta-[(5-methyl-2-)]	82	Lysine	59	0.766	0.920	7.366	0.570	3	139	2	140	2	12 duplicate
16501	77 [826; beta-[(5-methyl-2-)]	59	Omithine; Arginine	62	0.757	0.912	15.969	0.544	4	138	4	138	19	15 duplicate
17268	77 [826; beta-[(5-methyl-2-)]	69	Arginine	59	0.746	0.891	10.913	0.597	5	137	8	134	8	4 duplicate
11234	77 [826; beta-[(5-methyl-2-)]	10	Glycine	62	0.746	0.839	12.632	0.508	6	136	15	127	14	32 duplicate
10296	77 [826; beta-[(5-methyl-2-)]	3	Ethanolamine	61	0.743	0.875	32.381	0.518	7	135	10	132	102	29 duplicate
15744	77 [826; beta-[(5-methyl-2-)]	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	43	0.717	0.887	41.999	0.649	8	134	9	133	135	1 duplicate
13844	77 [826; beta-[(5-methyl-2-)]	30	[815; Ethyl-3(2H)-thiophenone]	62	0.713	0.863	6.899	0.528	9	133	12	130	1	22 duplicate
14393	77 [826; beta-[(5-methyl-2-)]	37	Phenylalanine	62	0.712	0.902	11.736	0.576	10	132	7	135	10	10 duplicate
16094	77 [826; beta-[(5-methyl-2-)]	55	[612; 4-Aminobutyric acid (2TBS)]	43	0.679	0.825	44.982	0.607	11	131	16	126	139	3 duplicate
17121	77 [826; beta-[(5-methyl-2-)]	67	Citric acid	62	0.671	0.850	12.151	0.468	12	130	14	128	13	62 duplicate
13863	77 [826; beta-[(5-methyl-2-)]	32	[729; N,N-Dimethyllysine methyl ester]	62	0.667	0.917	32.106	0.587	13	129	3	139	99	9 duplicate
7922	77 [826; beta-[(5-methyl-2-)]	138	[748; D-Sedoheptulose-7-phosphate (7TMS)]	16	0.667	0.822	11.882	0.393	14	128	18	124	11	108 original
13971	77 [826; beta-[(5-methyl-2-)]	33	Methionine	62	0.651	0.761	24.125	0.475	15	127	21	121	58	59 duplicate

15471	77 [826; beta-[[[5-methyl-2-48	Asparagine	62	0.634	0.736	24.881	0.526	16	128	26	116	59	23 duplicate
17194	77 [826; beta-[[[5-methyl-2-68	[570; Hypoxanthine (2TMS)]	18	0.621	0.903	28.688	0.594	17	125	5	137	78	5 duplicate
10569	77 [826; beta-[[[5-methyl-2-5	Leucine	45	0.608	0.777	30.367	0.592	18	124	22	120	91	7 duplicate
14078	77 [826; beta-[[[5-methyl-2-34	Aspartic acid	62	0.602	0.773	10.144	0.462	19	123	23	119	5	69 duplicate
7881	77 [826; beta-[[[5-methyl-2-95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	49	0.597	0.660	40.470	0.398	20	122	33	109	132	104 original
16582	77 [826; beta-[[[5-methyl-2-60	Glycerol-3-phosphate	62	0.596	0.780	12.045	0.502	21	121	20	122	12	39 duplicate
11103	77 [826; beta-[[[5-methyl-2-9	Proline	61	0.573	0.860	8.809	0.544	22	120	13	129	4	16 duplicate
10971	77 [826; beta-[[[5-methyl-2-8	Isoleucine	54	0.537	0.746	16.720	0.519	23	119	25	117	23	28 duplicate
13754	77 [826; beta-[[[5-methyl-2-31	[622; Parabenic acid (2TMS)]	62	0.534	0.727	33.335	0.452	24	118	28	114	108	76 duplicate
15189	77 [826; beta-[[[5-methyl-2-45	Homocysteine	59	0.531	0.576	44.589	0.478	25	117	37	105	138	58 duplicate
7875	77 [826; beta-[[[5-methyl-2-89	[775; Dopamine (4TMS)]	34	0.519	0.683	31.170	0.566	26	116	31	111	93	13 original
10838	77 [826; beta-[[[5-methyl-2-7	Threonine	62	0.490	0.785	11.320	0.516	27	115	19	123	9	30 duplicate
12489	77 [826; beta-[[[5-methyl-2-20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	0.480	0.873	35.085	0.843	28	114	11	131	113	2 duplicate
10158	77 [826; beta-[[[5-methyl-2-2	Serine	61	0.477	0.822	16.328	0.570	29	113	17	125	22	11 duplicate
16682	77 [826; beta-[[[5-methyl-2-61	[NA]	62	0.458	0.451	27.227	0.403	30	112	44	98	73	89 duplicate
7917	77 [826; beta-[[[5-methyl-2-131	[626; 5-Methylthioadenosine (3TMS)]	54	0.444	0.409	38.654	0.451	31	111	47	95	130	77 original
17047	77 [826; beta-[[[5-methyl-2-66	Glyceric acid-3-phosphate	62	0.424	0.722	29.486	0.506	32	110	29	113	86	34 duplicate
15563	77 [826; beta-[[[5-methyl-2-49	[877; Pyrophosphoric acid (4TMS)]	62	0.419	0.421	41.801	0.433	33	109	46	96	134	84 duplicate
12846	77 [826; beta-[[[5-methyl-2-23	Homoserine	62	0.405	0.704	24.482	0.542	34	108	30	112	58	17 duplicate
13308	77 [826; beta-[[[5-methyl-2-27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	52	0.347	0.735	36.875	0.539	35	107	27	115	124	18 duplicate
13079	77 [826; beta-[[[5-methyl-2-25	[709; 2,5-Diaminovalerolactam (2TMS)]	46	0.339	0.638	25.251	0.434	36	106	35	107	61	82 duplicate
7884	77 [826; beta-[[[5-methyl-2-98	[597; Ribose-5-phosphate methoxyamine (5TMS)]	47	0.330	0.583	38.132	0.510	37	105	36	108	129	31 original
7894	77 [826; beta-[[[5-methyl-2-108	Octadecenoic acid	62	0.329	0.432	30.283	0.367	38	104	45	97	90	123 original
17407	77 [826; beta-[[[5-methyl-2-71	[731; Erythrose (3TMS)]	62	0.327	0.565	20.027	0.453	39	103	38	104	35	75 duplicate
15833	77 [826; beta-[[[5-methyl-2-52	[NA]	44	0.317	0.460	35.951	0.523	40	102	43	99	120	26 duplicate
17677	77 [826; beta-[[[5-methyl-2-75	Lysine	62	0.313	0.759	15.851	0.545	41	101	24	118	17	14 duplicate
14289	77 [826; beta-[[[5-methyl-2-36	[596; N-Acetylglutamic acid (2TMS)]	62	0.304	0.640	10.444	0.504	42	100	34	108	6	38 duplicate
7910	77 [826; beta-[[[5-methyl-2-124	[734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecenoylethanol (1TMS)]	57	0.268	0.469	46.209	0.358	43	99	42	100	140	125 original
14996	77 [826; beta-[[[5-methyl-2-43	[548; Leucine (2TBS)]	58	0.240	0.311	25.497	0.421	44	98	49	93	64	90 duplicate
16819	77 [826; beta-[[[5-methyl-2-63	Glutamine	50	0.211	0.521	28.841	0.467	45	97	39	103	79	63 duplicate
16419	77 [826; beta-[[[5-methyl-2-58	[636; 4R-Acetalamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	62	0.210	0.665	16.212	0.483	46	96	32	110	20	53 duplicate
7893	77 [826; beta-[[[5-methyl-2-107	9-(Z)-Octadecenoic acid	62	0.201	0.281	18.829	0.343	47	94	51	91	27	131 original
7905	77 [826; beta-[[[5-methyl-2-119	[931; myo-Inositol-2-phosphate (7TMS)]	62	0.201	0.221	26.496	0.377	48	95	54	88	68	113 original
7923	77 [826; beta-[[[5-methyl-2-137	Ergosterol	62	0.186	0.297	21.315	0.350	49	93	50	92	41	130 original
7916	77 [826; beta-[[[5-methyl-2-130	Trehalose	61	0.160	0.327	12.911	0.339	50	92	48	94	16	132 original
7927	77 [826; beta-[[[5-methyl-2-141	Lanosta-8,24-dien-3-beta-ol	59	0.091	0.093	38.080	0.372	51	91	56	86	128	118 original
7924	77 [826; beta-[[[5-methyl-2-138	[674; Ergosterol (1TMS)]	44	0.089	0.238	35.783	0.355	52	90	52	90	117	128 original
7897	77 [826; beta-[[[5-methyl-2-111	[583; Erythritol (4TMS)]	40	0.082	0.084	38.914	0.307	53	89	57	85	125	139 original
7925	77 [826; beta-[[[5-methyl-2-139	[700; Ergosta-5,7-dien-3-ol]	36	0.063	0.177	36.054	0.309	54	88	55	87	121	138 original
7880	77 [826; beta-[[[5-methyl-2-94	Hexadecanoic acid	62	0.057	0.084	16.747	0.375	55	87	58	84	24	115 original
10433	77 [826; beta-[[[5-methyl-2-4	Phosphoric acid	51	0.054	0.518	10.639	0.465	56	86	40	102	7	87 duplicate
7895	77 [826; beta-[[[5-methyl-2-109	Octadecanoic acid	62	0.039	-0.003	20.365	0.372	57	85	59	83	36	119 original
7919	77 [826; beta-[[[5-methyl-2-133	[855; Squalene]	62	0.019	0.228	27.077	0.361	58	84	53	89	71	122 original
7876	77 [826; beta-[[[5-methyl-2-90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	62	0.009	-0.027	26.756	0.361	59	83	60	82	69	124 original
7869	77 [826; beta-[[[5-methyl-2-83	Sorbitol	57	0.008	0.477	12.859	0.502	60	82	41	101	15	40 original
16896	77 [826; beta-[[[5-methyl-2-64	[789; Tyramine (3TMS)]	61	-0.015	-0.059	28.914	0.338	61	81	64	78	80	133 duplicate
7879	77 [826; beta-[[[5-methyl-2-93	[607; Putrescine (4TMS)]	58	-0.022	-0.337	40.316	0.423	62	80	76	66	131	89 original
7926	77 [826; beta-[[[5-methyl-2-140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	47	-0.025	-0.054	38.075	0.378	63	79	63	79	127	112 original

77	[826; beta-[[[5-methyl-2- 72	[918; D-Xylopyranose (4TMS)]	62	-0.039	-0.033	31,794	0.373	64	78	61	81	98	116
77	[826; beta-[[[5-methyl-2- 15	Alanine	62	-0.085	-0.189	19,209	0.484	65	77	68	74	29	51
77	[826; beta-[[[5-methyl-2- 118	[777; Fructopyranose-6-phosphate (6TMS)]	57	-0.088	-0.191	29,874	0.335	66	75	69	73	87	134
77	[826; beta-[[[5-methyl-2- 127	[777; Fructose-6-phosphate methoxamine (6TMS)]	36	-0.096	-0.267	18,122	0.269	67	76	73	69	25	141
77	[826; beta-[[[5-methyl-2- 84	Mannitol	60	-0.098	-0.634	22,347	0.495	68	74	106	36	46	41
77	[826; beta-[[[5-methyl-2- 53	Glycerol-2-phosphate	62	-0.106	-0.210	35,799	0.331	69	73	70	72	118	136
77	[826; beta-[[[5-methyl-2- 126	[559; Erythritol (4TMS)]	43	-0.134	-0.043	22,532	0.411	70	72	62	80	47	94
77	[826; beta-[[[5-methyl-2- 96	myo-Inositol	48	-0.137	-0.158	42,479	0.358	71	71	66	76	138	126
77	[826; beta-[[[5-methyl-2- 79	Glucose	62	-0.139	-0.391	19,522	0.465	72	70	81	61	32	66
135													
77	[826; beta-[[[5-methyl-2- 135	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	62	-0.150	-0.235	20,951	0.356	73	69	72	70	39	127
77	[826; beta-[[[5-methyl-2- 123	[945; Galacturanoose-6-phosphate (7TMS)]	62	-0.151	-0.171	22,961	0.474	74	68	67	75	50	60
77	[826; beta-[[[5-methyl-2- 114	Fructose-6-phosphate	51	-0.178	-0.405	30,623	0.448	75	67	84	58	92	78
77	[826; beta-[[[5-methyl-2- 116	[882; Pseudouridine (5TMS)]	30	-0.200	-0.115	25,824	0.393	76	66	65	77	68	110
77	[826; beta-[[[5-methyl-2- 113	Galactose-6-phosphate	60	-0.215	-0.466	32,977	0.440	77	65	89	53	105	79
77	[826; beta-[[[5-methyl-2- 85	[529; Methylcitric acid (4TMS)]	48	-0.248	-0.394	28,384	0.525	78	64	82	60	77	25
77	[826; beta-[[[5-methyl-2- 41	[639; Proline (2TMS)]	62	-0.254	-0.219	21,143	0.408	79	63	71	71	40	96
77	[826; beta-[[[5-methyl-2- 102	[904; Galactose methoxamine (5TMS)]	62	-0.258	-0.367	31,346	0.399	80	62	77	65	94	102
77	[826; beta-[[[5-methyl-2- 74	[912; Tetradecanoic acid (1TMS)]	62	-0.264	-0.268	32,454	0.460	81	61	74	68	103	71
77	[826; beta-[[[5-methyl-2- 47	[NA]	62	-0.266	-0.423	31,379	0.403	82	60	86	56	95	100
77	[826; beta-[[[5-methyl-2- 112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (8TMS)]	61	-0.274	-0.400	41,389	0.395	83	59	83	59	133	107
77	[826; beta-[[[5-methyl-2- 100	[857; Mannitol (6TMS)]	62	-0.276	-0.487	25,359	0.438	84	58	93	49	63	81
77	[826; beta-[[[5-methyl-2- 104	[795; Erythritol (4TMS)]	61	-0.284	-0.291	29,471	0.471	85	57	75	67	84	61
77	[826; beta-[[[5-methyl-2- 104	[795; Erythritol (4TMS)]	48	-0.289	-0.373	23,004	0.372	86	58	78	64	51	117
77	[826; beta-[[[5-methyl-2- 44	[910; 2-Ketogluconic acid methoxamine (4TMS)]	43	-0.289	-0.477	19,996	0.279	87	55	91	51	34	140
77	[826; beta-[[[5-methyl-2- 128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	62	-0.300	-0.378	26,253	0.395	88	54	79	63	67	105
77	[826; beta-[[[5-methyl-2- 121	[590; 1-Acetyl-2-thiohydantoin]	41	-0.305	-0.615	32,607	0.330	89	53	102	104	137	136
77	[826; beta-[[[5-methyl-2- 132	[895; Isomaltose methoxamine (8TMS)]	62	-0.341	-0.388	24,163	0.395	90	52	80	62	57	106
77	[826; beta-[[[5-methyl-2- 19	Alanine (BP) (3TMS)	62	-0.341	-0.388	24,163	0.395	90	52	80	62	57	106
77	[826; beta-[[[5-methyl-2- 122	[644; Erythritol (4TMS)]	52	-0.349	-0.475	34,993	0.398	91	51	90	52	112	103
77	[826; beta-[[[5-methyl-2- 110	[715; Erythritol (4TMS)]	50	-0.371	-0.482	31,454	0.467	92	50	92	57	97	65
77	[826; beta-[[[5-methyl-2- 121	[657; Erythritol (4TMS)]	53	-0.380	-0.405	35,449	0.389	93	49	85	57	116	108
77	[826; beta-[[[5-methyl-2- 117	[724; Glycerol (3TMS)]	54	-0.384	-0.457	29,473	0.405	94	48	88	54	85	98
77	[826; beta-[[[5-methyl-2- 115	Glucose-6-phosphate	60	-0.400	-0.593	18,642	0.418	95	47	98	44	28	93
77	[826; beta-[[[5-methyl-2- 35	Pyroglutamic acid	62	-0.403	-0.617	21,819	0.455	96	46	104	38	44	73
77	[826; beta-[[[5-methyl-2- 97	[756; beta-D-Methylglucopyranoside (4TMS)]	50	-0.407	-0.753	25,536	0.434	97	45	123	19	65	83
77	[826; beta-[[[5-methyl-2- 105	[705; 2-Ketogluconic acid (5TMS)]	46	-0.432	-0.689	23,324	0.382	99	43	112	30	54	111
77	[826; beta-[[[5-methyl-2- 91	[766; beta-D-Methylglucopyranoside (4TMS)]	62	-0.443	-0.728	35,353	0.477	100	42	118	24	115	57
77	[826; beta-[[[5-methyl-2- 26	Citramalic acid	62	-0.452	-0.593	18,359	0.427	101	41	97	45	26	87
77	[826; beta-[[[5-methyl-2- 73	[708; Glucose methoxamine (5TMS)]	56	-0.456	-0.526	34,471	0.497	102	40	94	48	110	41
77	[826; beta-[[[5-methyl-2- 80	[772; D-Glucose (5TMS)]	60	-0.459	-0.599	22,660	0.375	103	39	99	43	48	114
77	[826; beta-[[[5-methyl-2- 12	Glycric acid	61	-0.461	-0.720	36,528	0.459	104	38	117	25	122	72
77	[826; beta-[[[5-methyl-2- 6	Glycerol	62	-0.464	-0.621	21,748	0.408	105	37	105	37	43	97
77	[826; beta-[[[5-methyl-2- 28	Malic acid	62	-0.465	-0.695	25,082	0.508	106	36	113	28	60	33
77	[826; beta-[[[5-methyl-2- 40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	62	-0.490	-0.617	16,275	0.486	107	35	103	39	21	48
77	[826; beta-[[[5-methyl-2- 40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	52	-0.498	-0.559	19,403	0.497	108	34	96	46	31	42
77	[826; beta-[[[5-methyl-2- 120	[945; Uridine (3TMS)]	50	-0.499	-0.712	35,339	0.419	109	33	114	28	114	91
77	[826; beta-[[[5-methyl-2- 22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	-0.501	-0.616	27,778	0.331	110	32	102	40	75	135
77	[826; beta-[[[5-methyl-2- 92	[680; Glycerol-2-phosphate (4TMS)]	62	-0.501	-0.719	31,440	0.484	111	31	116	26	96	52
77	[826; beta-[[[5-methyl-2- 101	[832; Dopamine (4TMS)]	62	-0.508	-0.671	23,126	0.427	112	30	108	34	52	86
77	[826; beta-[[[5-methyl-2- 76	Fructose	62	-0.508	-0.681	19,971	0.462	113	29	110	32	33	70
77	[826; beta-[[[5-methyl-2- 21	[878; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	62	-0.508	-0.681	19,971	0.462	113	29	110	32	33	70
77	[826; beta-[[[5-methyl-2- 103	[648; Ethylamine (2TMS)]	61	-0.518	-0.739	32,202	0.482	114	28	121	21	101	54

7892	77 [826; beta-[[5-methyl-2-106 [733; Threitol (4TMS)]	60 -0.519	-0.616	29.954	0.519	115	27	101	41	88	27 original
10019	77 [826; beta-[[5-methyl-2-1 [938; Sulfuric acid (2TMS)]	34 -0.529	-0.717	20.764	0.353	116	26	115	27	37	129 duplicate
7864	77 [826; beta-[[5-methyl-2-78 Mannose	60 -0.531	-0.655	35.856	0.424	117	25	107	35	119	88 original
11748	77 [826; beta-[[5-methyl-2-14 Fumaric acid	62 -0.540	-0.735	34.877	0.504	118	24	119	23	111	37 duplicate
14496	77 [826; beta-[[5-methyl-2-38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	62 -0.553	-0.775	27.944	0.487	119	23	126	18	76	64 duplicate
7911	77 [826; beta-[[5-methyl-2-125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	62 -0.564	-0.887	22.757	0.454	120	22	111	31	49	74 original
7873	77 [826; beta-[[5-methyl-2-87 [945; beta-D-Glucopyranose (5TMS)]	60 -0.573	-0.677	24.033	0.403	121	21	109	33	55	101 original
11364	77 [826; beta-[[5-methyl-2-11 Succinic acid	62 -0.575	-0.742	26.995	0.464	122	20	122	20	70	68 duplicate
17337	77 [826; beta-[[5-methyl-2-70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	56 -0.578	-0.428	19.216	0.440	123	19	87	55	30	80 duplicate
13533	77 [826; beta-[[5-methyl-2-29 Erythritol	62 -0.582	-0.808	30.093	0.528	124	18	128	14	89	24 duplicate
7885	77 [826; beta-[[5-methyl-2-99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	39 -0.598	-0.766	27.709	0.418	125	17	125	17	74	92 original
16741	77 [826; beta-[[5-methyl-2-62 [812; D-Xylofuranose (4TMS)]	62 -0.612	-0.738	21.473	0.432	126	16	120	22	42	85 duplicate
16008	77 [826; beta-[[5-methyl-2-54 [NA]	53 -0.614	-0.765	34.067	0.369	127	15	124	18	109	120 duplicate
12123	77 [826; beta-[[5-methyl-2-17 [700; 2-methyl-1,2-propanediol (2TMS)]	62 -0.647	-0.809	23.220	0.498	128	14	129	13	53	43 duplicate
16336	77 [826; beta-[[5-methyl-2-57 [757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	53 -0.656	-0.787	29.457	0.409	129	13	127	15	83	95 duplicate
7874	77 [826; beta-[[5-methyl-2-88 Gluconic acid	62 -0.658	-0.824	29.074	0.505	130	12	134	8	81	35 original
14598	77 [826; beta-[[5-methyl-2-39 [829; 1-Phenylethanol (1TMS)]	61 -0.660	-0.811	29.287	0.491	131	11	130	12	82	46 duplicate
16252	77 [826; beta-[[5-methyl-2-56 [829; Orotic acid (3TMS)]	62 -0.669	-0.824	36.863	0.480	132	10	133	9	123	55 duplicate
7920	77 [826; beta-[[5-methyl-2-134 Isomaltose	62 -0.674	-0.835	27.116	0.485	133	9	136	6	72	50 original
7872	77 [826; beta-[[5-methyl-2-86 [793; D-Galactono-1,4-lactone (4TMS)]	59 -0.681	-0.820	33.209	0.489	134	8	132	10	107	47 original
7915	77 [826; beta-[[5-methyl-2-129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	57 -0.682	-0.819	33.044	0.485	135	7	131	11	106	49 original
11999	77 [826; beta-[[5-methyl-2-16 [644; 2-Methyl-1,3-butanediol (2TMS)]	62 -0.683	-0.856	21.908	0.539	136	6	140	2	45	19 duplicate
12963	77 [826; beta-[[5-methyl-2-24 [725; 2-Ketocacetic acid (2TMS)]	62 -0.684	-0.854	20.892	0.505	137	5	138	4	38	36 duplicate
16972	77 [826; beta-[[5-methyl-2-65 [846; 3-Deoxyglucitol (5TMS)]	61 -0.702	-0.825	38.015	0.476	138	4	135	7	126	58 duplicate
15284	77 [826; beta-[[5-methyl-2-46 Arabinose	62 -0.719	-0.837	32.179	0.493	139	3	137	5	100	45 duplicate
15854	77 [826; beta-[[5-methyl-2-50 [746; Ribonic acid-1,4-lactone (3TMS)]	59 -0.722	-0.855	43.570	0.530	140	2	139	3	137	21 duplicate
11821	77 [826; beta-[[5-methyl-2-13 Uridil	62 -0.740	-0.863	25.289	0.539	141	1	141	1	62	20 duplicate
17743	78 Mannose	62 0.728	0.901	25.508	0.614	1	141	1	141	114	5 duplicate
7955	78 Mannose	60 0.701	0.891	8.481	0.643	2	140	2	140	19	2 original
7935	78 Mannose	59 0.677	0.885	18.499	0.602	3	139	3	139	82	7 original
14185	78 Mannose	62 0.660	0.882	43.266	0.578	4	138	4	138	139	22 duplicate
14700	78 Mannose	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	62 0.657	0.835	37.274	0.592	5	137	11	131	16 duplicate
7970	78 Mannose	121 [657; Erythritol (4TMS)]	53 0.650	0.827	8.431	0.575	6	136	17	125	25
17545	78 Mannose	73 [708; Glucose methoxyamine (5TMS)]	56 0.649	0.801	6.288	0.541	7	135	27	115	8
7964	78 Mannose	115 Glucose-6-phosphate	60 0.643	0.867	25.695	0.573	8	134	5	137	115
7959	78 Mannose	110 [715; Erythritol (4TMS)]	52 0.637	0.861	6.322	0.647	9	133	6	136	9
14497	78 Mannose	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	62 0.629	0.825	9.858	0.556	10	132	18	124	30
7966	78 Mannose	117 [724; Glycerol (3TMS)]	54 0.628	0.811	5.532	0.593	11	131	23	119	2
7971	78 Mannose	122 [644; Erythritol (4TMS)]	50 0.618	0.818	11.000	0.582	12	130	21	121	35
13422	78 Mannose	28 Malic acid	62 0.617	0.827	12.277	0.577	13	129	16	126	43
16742	78 Mannose	62 [812; D-Xylofuranose (4TMS)]	62 0.615	0.848	16.706	0.557	14	128	10	132	73
11749	78 Mannose	14 Fumaric acid	62 0.613	0.817	7.694	0.525	15	127	22	120	15
14599	78 Mannose	39 [829; 1-Phenylethanol (1TMS)]	61 0.610	0.833	14.781	0.571	16	126	12	130	62
12964	78 Mannose	24 [725; 2-Ketocacetic acid (2TMS)]	62 0.602	0.828	33.545	0.604	17	125	15	127	126
7983	78 Mannose	134 Isomaltose	62 0.599	0.851	24.439	0.597	18	124	9	133	110
7974	78 Mannose	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	62 0.591	0.831	32.463	0.546	19	123	13	129	122
12000	78 Mannose	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	62 0.589	0.785	19.538	0.597	20	122	29	113	80
15285	78 Mannose	46 Arabinose	62 0.585	0.851	14.911	0.587	21	121	8	134	63
16973	78 Mannose	65 [646; 3-Deoxyglucitol (5TMS)]	61 0.580	0.858	7.568	0.595	22	120	7	135	14

7937	78 Mannose	88	Gluconic acid	0.775	11,911	0.581	23	119	31	111	40	20 original
15094	78 Mannose	48	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	0.806	8,399	0.636	24	118	25	117	10	3 duplicate
15655	78 Mannose	59	[746; Ribonic acid-1,4-lactone (3TMS)]	0.779	14,052	0.528	25	117	30	112	58	50 duplicate
16253	78 Mannose	62	[829; Orolic acid (3TMS)]	0.829	6,278	0.590	26	116	14	128	7	12 duplicate
7962	78 Mannose	60	Galactose-6-phosphate	0.824	5,685	0.519	27	115	20	122	3	55 original
11622	78 Mannose	62	Uracil	0.798	16,965	0.597	28	114	28	114	77	10 duplicate
13534	78 Mannose	62	Erythritol	0.762	8,833	0.525	29	113	34	108	23	53 duplicate
17338	78 Mannose	56	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	0.659	20,891	0.467	30	112	50	92	89	89 duplicate
11365	78 Mannose	62	Succinic acid	0.766	10,761	0.493	31	111	33	109	33	70 duplicate
7978	78 Mannose	57	[940; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	0.825	7,440	0.573	32	110	19	123	13	26 original
7953	78 Mannose	61	[795; Erythritol (4TMS)]	0.732	8,367	0.509	33	109	38	104	18	63 original
12729	78 Mannose	50	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	0.733	8,170	0.524	34	108	37	105	16	54 duplicate
10705	78 Mannose	62	Glycerol	0.771	44,005	0.537	35	107	32	110	140	48 duplicate
12124	78 Mannose	62	[700; 2-methyl-1,2-propanediol (2TMS)]	0.761	18,944	0.495	36	106	35	107	87	68 duplicate
7963	78 Mannose	51	Fructose-6-phosphate	0.808	6,019	0.566	37	105	24	118	5	31 original
7975	78 Mannose	43	[559; Erythritol (4TMS)]	0.699	6,036	0.588	38	104	42	100	6	13 original
12610	78 Mannose	62	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	0.689	19,319	0.484	39	103	46	96	88	78 duplicate
13195	78 Mannose	62	Citramalic acid	0.704	19,659	0.483	40	102	40	102	93	81 duplicate
12369	78 Mannose	62	Alanine (BP) (3TMS)	0.755	13,491	0.516	41	101	36	106	49	57 duplicate
7951	78 Mannose	62	[904; Galactose methoxyamine (5TMS)]	0.610	8,726	0.461	42	100	55	87	21	96 original
7949	78 Mannose	62	[857; Mannitol (5TMS)]	0.648	12,238	0.486	43	99	51	91	42	76 original
11494	78 Mannose	61	Glyceric acid	0.689	8,840	0.497	44	98	45	97	24	67 duplicate
16337	78 Mannose	53	[757; 2-Deoxy-pentose-3-yose dimethoxyamine (2TMS)]	0.801	10,338	0.568	45	97	26	116	31	30 duplicate
7972	78 Mannose	62	[945; Galacturonic acid-6-phosphate (7TMS)]	0.679	13,760	0.493	47	95	47	95	56	71 original
7852	78 Mannose	61	[648; Ethylamine (2TMS)]	0.598	13,577	0.489	48	94	57	85	52	73 original
17612	78 Mannose	62	[912; Tetradecanoic acid (1TMS)]	0.674	8,335	0.558	49	93	48	94	17	35 duplicate
7869	78 Mannose	52	[945; Uridine (3TMS)]	0.283	13,725	0.512	50	92	72	70	55	61 original
7961	78 Mannose	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	0.593	13,859	0.468	51	91	58	84	54	88 original
12247	78 Mannose	61	[590; 1-Acetyl-2-thiohydantoin]	0.584	11,310	0.475	52	90	59	83	36	86 duplicate
16009	78 Mannose	62	[NA]	0.701	8,594	0.516	53	89	41	101	20	58 duplicate
7941	78 Mannose	92	[680; Glycerol-2-phosphate (4TMS)]	0.665	6,734	0.551	54	88	49	93	12	41 original
7981	78 Mannose	52	[895; Isomaltose methoxyamine (8TMS)]	0.692	12,301	0.564	55	87	44	98	44	32 original
7934	78 Mannose	47	[529; Methylictric acid (4TMS)]	0.608	9,443	0.477	56	86	56	86	26	84 original
14800	78 Mannose	62	[639; Proline (2TMS)]	0.579	16,524	0.491	57	85	60	82	71	72 duplicate
7936	78 Mannose	60	[845; beta-D-Glucopyranose (5TMS)]	0.719	36,141	0.480	58	84	39	103	132	83 original
7984	78 Mannose	62	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	0.492	16,305	0.413	59	83	63	79	69	115 original
7950	78 Mannose	62	[832; Dopamine (4TMS)]	0.474	12,044	0.430	60	82	65	77	41	107 original
7928	78 Mannose	62	Glucose	0.694	36,577	0.504	61	81	43	99	133	64 original
7932	78 Mannose	57	Sorbitol	-0.013	25,213	0.338	62	80	87	55	112	139 original
7977	78 Mannose	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	0.578	6,715	0.549	63	79	61	81	11	42 original
7940	78 Mannose	91	[766; beta-D-Methylglucopyranoside (4TMS)]	0.389	17,316	0.420	64	78	69	73	79	111 original
7965	78 Mannose	62	[892; Pseudouridine (5TMS)]	0.267	9,760	0.485	65	77	75	67	29	77 original
7948	78 Mannose	30	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	0.626	8,746	0.553	66	76	53	89	22	39 original
16897	78 Mannose	40	[254]	0.409	9,692	0.380	67	75	68	74	28	125 duplicate
7946	78 Mannose	61	[789; Tyramine (3TMS)]	0.469	19,398	0.463	68	74	66	76	89	93 original
11875	78 Mannose	50	[756; beta-D-Methylglucopyranoside (4TMS)]	0.480	20,844	0.531	69	73	64	78	98	49 duplicate
7954	78 Mannose	62	Alanine	0.376	10,942	0.581	70	72	70	72	34	19 original
7960	78 Mannose	46	[705; 2-Ketogluconic acid (5TMS)]	0.352	18,220	0.483	71	71	71	71	81	82 original
		40	[583; Erythritol (4TMS)]	0.228								

7929	78 Mannose	80 [772; D-Glucose (5TMS)]	60	0.226	0.621	32.040	0.445	72	70	54	88	121	104 original
7982	78 Mannose	133 [855; Squalene]	62	0.226	0.239	11.889	0.413	73	69	76	68	39	116 original
7945	78 Mannose	96 myo-Inositol	49	0.214	0.154	16.201	0.285	74	68	79	63	68	141 original
7958	78 Mannose	109 Octadecanoic acid	62	0.201	0.532	23.836	0.553	75	67	62	80	108	38 original
7987	78 Mannose	138 [674; Ergosterol (1TMS)]	46	0.179	0.269	14.061	0.477	76	66	74	68	59	85 original
7943	78 Mannose	94 Hexadecanoic acid	62	0.114	0.421	24.370	0.515	77	65	87	75	109	60 original
7989	78 Mannose	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49	0.111	0.135	13.874	0.455	78	64	80	62	57	101 original
7990	78 Mannose	141 Lanosta-8,24-dien-3-beta-ol	60	0.098	0.109	12.809	0.461	79	63	82	60	46	97 original
7976	78 Mannose	127 [777; Fructose-6-phosphate methoxymine (6TMS)]	37	0.081	0.235	5.870	0.581	80	62	77	65	4	18 original
7985	78 Mannose	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.059	0.272	3.585	0.484	81	61	73	68	1	79 original
17408	78 Mannose	71 [731; Erythrose (3TMS)]	62	0.036	-0.007	16.731	0.423	82	60	84	58	75	109 duplicate
7986	78 Mannose	137 Ergosterol	62	0.023	-0.009	18.918	0.486	83	59	85	57	86	75 original
7967	78 Mannose	118 [928; Glucopyranose-6-phosphate (6TMS)]	56	0.003	0.227	10.637	0.421	84	58	78	64	32	110 original
7933	78 Mannose	84 Mannitol	60	-0.018	0.124	34.654	0.369	85	57	81	61	128	127 original
15379	78 Mannose	47 [NA]	62	-0.025	-0.011	14.987	0.457	86	56	86	56	64	99 duplicate
7973	78 Mannose	124 [734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]	57	-0.056	-0.217	20.182	0.414	87	55	97	45	94	114 original
7942	78 Mannose	93 [607; Putrescine (4TMS)]	58	-0.074	-0.066	15.709	0.381	88	54	88	54	67	124 original
7979	78 Mannose	130 Trehalose	61	-0.081	-0.152	33.182	0.347	89	53	80	52	125	136 original
7968	78 Mannose	119 [931; myo-Inositol-2-phosphate (7TMS)]	62	-0.083	-0.180	14.237	0.453	90	52	92	50	60	102 original
10434	78 Mannose	4 Phosphoric acid	50	-0.086	-0.150	36.975	0.353	91	51	89	53	134	134 duplicate
15922	78 Mannose	53 Glycerol-2-phosphate [636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	62	-0.097	-0.187	11.788	0.323	92	50	94	48	38	140 duplicate
16420	78 Mannose	58 (1TMS)]	62	-0.099	-0.216	21.112	0.368	93	49	96	46	102	129 duplicate
14290	78 Mannose	38 [596; N-Acetylglutamic acid (2TMS)]	62	-0.107	-0.185	32.584	0.418	94	48	93	49	123	113 duplicate
10020	78 Mannose	1 [938; Sulfuric acid (2TMS)]	35	-0.123	-0.003	9.559	0.560	95	47	83	59	27	34 duplicate
7988	78 Mannose	139 [700; Ergosta-5,7-dien-3-ol]	38	-0.127	-0.174	16.697	0.354	96	46	91	51	72	133 original
17678	78 Mannose	75 Lysine	62	-0.130	-0.271	43.121	0.342	97	45	99	43	138	138 duplicate
7939	78 Mannose	90 [910; 9-(Z)-Hexadecanoic acid (1TMS)]	62	-0.155	-0.225	13.562	0.381	98	44	98	44	51	130 original
7956	78 Mannose	107 9-(Z)-Octadecanoic acid	62	-0.177	-0.317	19.620	0.382	99	43	100	42	91	123 original
17477	78 Mannose	72 [919; D-Xylopyranose (4TMS)]	61	-0.186	-0.211	13.543	0.358	100	42	95	47	50	132 duplicate
17048	78 Mannose	66 Glyceral acid-3-phosphate	62	-0.187	-0.317	11.730	0.399	101	41	101	41	37	119 duplicate
10839	78 Mannose	7 Threonine	62	-0.196	-0.332	33.926	0.352	102	40	103	39	127	135 duplicate
10159	78 Mannose	2 Serine	60	-0.241	-0.368	24.874	0.358	103	39	104	38	111	131 duplicate
17122	78 Mannose	67 Citric acid	62	-0.273	-0.443	27.838	0.399	104	38	108	34	119	120 duplicate
13309	78 Mannose	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	51	-0.278	-0.613	20.968	0.464	105	37	115	27	100	92 duplicate
16583	78 Mannose	60 Glycerol-3-phosphate	62	-0.289	-0.417	26.012	0.445	106	36	105	37	117	103 duplicate
7957	78 Mannose	108 Octadecanoic acid	62	-0.300	-0.425	12.909	0.432	107	35	106	36	47	108 original
14897	78 Mannose	43 [548; Leucine (2TBS)]	58	-0.316	-0.463	14.572	0.488	108	34	109	33	61	74 duplicate
12847	78 Mannose	23 Homoserine	62	-0.327	-0.673	18.627	0.484	109	33	123	19	84	80 duplicate
7947	78 Mannose	98 [697; Ribose-5-phosphate methoxymine (5TMS)]	46	-0.328	-0.631	18.105	0.465	110	32	118	24	80	91 original
13755	78 Mannose	31 [622; Parabanic acid (2TMS)]	62	-0.328	-0.486	13.638	0.474	111	31	110	32	53	87 duplicate
11104	78 Mannose	9 Proline	61	-0.354	-0.435	33.167	0.368	112	30	107	35	124	128 duplicate
10972	78 Mannose	8 Isoleucine	53	-0.356	-0.320	23.822	0.344	113	29	102	40	107	137 duplicate
14394	78 Mannose	37 Phenylalanine	62	-0.357	-0.521	27.115	0.419	114	28	111	31	118	112 duplicate
13080	78 Mannose	25 [709; 2,5-Diaminovalerolactam (2TMS)]	46	-0.405	-0.688	18.601	0.552	115	27	126	16	83	40 duplicate
15834	78 Mannose	52 [NA]	45	-0.414	-0.716	21.305	0.502	116	26	129	13	104	65 duplicate
15663	78 Mannose	61 [NA]	62	-0.420	-0.530	13.176	0.463	117	25	112	30	48	95 duplicate
10297	78 Mannose	3 Ethanolamine	60	-0.442	-0.690	15.455	0.516	118	24	127	15	65	56 duplicate
16820	78 Mannose	63 Glutamine	51	-0.448	-0.788	22.715	0.561	119	23	134	8	106	33 duplicate
14079	78 Mannose	34 Aspartic acid	62	-0.466	-0.615	37.442	0.463	120	22	116	26	136	94 duplicate



17195	78 Mannose	68 [570; Hypoxanthine (2TMS)]	20 -0.474	-0.831	12.807	0.460	121	21	137	5	45	98 duplicate
13864	78 Mannose	32 [728; N,N-Dimethyllysine methyl ester]	61 -0.480	-0.642	21.019	0.525	122	20	119	23	101	51 duplicate
15472	78 Mannose	48 Asparagine	62 -0.488	-0.798	20.286	0.543	123	19	135	7	98	46 duplicate
15745	78 Mannose	51 [498; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	43 -0.488	-0.622	18.983	0.398	124	18	117	25	76	122 duplicate
16502	78 Mannose	59 Ornithine; Arginine	62 -0.503	-0.594	44.779	0.399	125	17	113	29	141	123 duplicate
7930	78 Mannose	81 Tyrosine	62 -0.513	-0.697	39.386	0.546	126	16	128	14	137	44 original
15190	78 Mannose	45 Homocysteine	59 -0.528	-0.687	19.743	0.443	127	15	125	17	92	105 duplicate
11235	78 Mannose	10 Glycine	62 -0.528	-0.824	25.728	0.580	128	14	138	6	116	21 duplicate
17807	78 Mannose	[826; beta-[(5-methyl-2-thienyl)methyl]phenylamino-benzeneacetic acid methyl ester]	60 -0.531	-0.655	35.856	0.424	129	13	121	21	130	108 duplicate
7980	78 Mannose	131 [626; 5-Methylthioadenosine (3TMS)]	53 -0.533	-0.744	16.722	0.589	130	12	131	11	74	29 original
17267	78 Mannose	69 Arginine	58 -0.537	-0.729	28.228	0.511	131	11	130	12	120	62 duplicate
7844	78 Mannose	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	48 -0.537	-0.764	17.158	0.457	132	10	133	9	78	100 original
13645	78 Mannose	30 [815; Ethyl-3(2H)-thiophenone]	62 -0.544	-0.643	35.343	0.400	133	8	120	22	129	118 duplicate
13972	78 Mannose	33 Methionine	62 -0.544	-0.662	18.695	0.466	134	9	122	20	85	90 duplicate
15564	78 Mannose	49 [877; Pyrophosphoric acid (4TMS)]	62 -0.556	-0.674	22.329	0.515	135	7	124	18	105	59 duplicate
14899	78 Mannose	42 Glutamic acid	58 -0.584	-0.604	36.070	0.375	136	6	114	28	131	126 duplicate
16095	78 Mannose	55 [612; 4-Aminobutyric acid (2TBS)]	42 -0.605	-0.839	20.535	0.494	137	5	138	4	97	69 duplicate
7938	78 Mannose	89 [775; Dopamine (4TMS)]	34 -0.611	-0.886	21.148	0.544	138	4	140	2	103	45 original
12490	78 Mannose	20 [619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	30 -0.614	-0.886	15.531	0.571	139	3	139	3	66	28 duplicate
10570	78 Mannose	5 Leucine	44 -0.634	-0.758	16.341	0.501	140	2	132	10	70	66 duplicate
7931	78 Mannose	82 Lysine	39 -0.679	-0.923	25.460	0.618	141	1	141	1	113	4 original
11876	79 Glucose	15 Alanine	64 -0.622	-0.867	17.846	0.584	1	141	4	138	26	33 duplicate
8034	79 Glucose	123 [945; Galactofuranose-6-phosphate (7TMS)]	64 -0.601	-0.881	25.623	0.596	2	140	5	137	52	26 original
8025	79 Glucose	114 Fructose-6-phosphate	53 -0.586	-0.889	33.730	0.598	3	139	1	141	87	24 original
16898	79 Glucose	64 [788; Tyramine (3TMS)]	63 -0.546	-0.725	34.010	0.439	4	138	14	128	91	108 duplicate
8015	79 Glucose	104 [795; Erythritol (4TMS)]	63 -0.534	-0.715	32.122	0.572	5	137	15	127	77	38 original
8024	79 Glucose	113 Galactose-6-phosphate	62 -0.489	-0.868	35.743	0.614	6	136	3	139	99	19 original
10708	79 Glucose	6 Glyceral	64 -0.458	-0.851	9.199	0.568	7	135	6	136	6	40 duplicate
12370	79 Glucose	19 Alanine (BP) (3TMS)	64 -0.437	-0.744	25.218	0.558	8	134	11	131	51	45 duplicate
17546	79 Glucose	73 [708; Glucose methoxamine (5TMS)]	57 -0.416	-0.692	34.621	0.503	9	133	17	125	98	72 duplicate
16421	79 Glucose	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	58 -0.412	-0.195	22.580	0.460	10	132	68	74	41	93 duplicate
7991	79 Glucose	80 [772; D-Glucose (5TMS)]	62 -0.366	-0.746	9.477	0.494	11	131	10	132	8	74 original
14801	79 Glucose	41 [639; Proline (2TMS)]	64 -0.360	-0.568	23.056	0.480	12	130	26	116	42	81 duplicate
17744	79 Glucose	78 Fructose	64 -0.340	-0.810	13.003	0.572	13	129	9	133	15	36 duplicate
8017	79 Glucose	106 [733; Threitol (4TMS)]	62 -0.332	-0.685	29.313	0.620	14	128	18	124	65	12 original
8036	79 Glucose	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64 -0.327	-0.878	6.917	0.572	15	127	2	140	1	37 original
14186	79 Glucose	35 Pyroglutamic acid	64 -0.320	-0.810	8.729	0.578	16	126	8	134	5	35 duplicate
17871	79 Glucose	78 Mannose	62 -0.320	-0.694	36.577	0.504	17	125	16	126	103	70 duplicate
17679	79 Glucose	75 Lysine	64 -0.317	-0.100	10.961	0.493	18	124	75	67	11	75 duplicate
8026	79 Glucose	115 Glucose-6-phosphate	62 -0.293	-0.810	11.105	0.584	19	123	7	135	12	32 original
14701	79 Glucose	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	64 -0.277	-0.515	7.520	0.536	20	122	30	112	2	54 duplicate
8041	79 Glucose	130 Trehalose	63 -0.264	-0.106	9.478	0.428	21	121	74	68	9	114 original
17339	79 Glucose	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57 -0.244	-0.658	16.536	0.543	22	120	19	123	21	49 duplicate
7997	79 Glucose	86 [793; D-Galactono-1,4-lactone (4TMS)]	61 -0.223	-0.740	24.925	0.612	23	119	12	130	50	21 original
7998	79 Glucose	87 [945; beta-D-Glucopyranose (5TMS)]	62 -0.223	-0.734	8.692	0.540	24	118	13	129	4	51 original
10160	79 Glucose	2 Serine	62 -0.221	-0.020	28.260	0.441	25	117	84	58	54	107 duplicate
7994	79 Glucose	83 Sorbitol	58 -0.214	-0.088	17.490	0.468	26	116	77	65	25	87 original
8029	79 Glucose	118 [926; Glucopyranose-6-phosphate (6TMS)]	58 -0.205	-0.407	35.731	0.426	27	115	43	99	98	115 original

8032	79 Glucose	121 [657; Erythritol (4TMS)]	55	0.195	0.473	42.367	0.539	28	114	34	108	122	53 original
17049	79 Glucose	66 Glyceric acid-3-phosphate	64	0.194	0.018	35.987	0.492	29	113	82	80	102	76 duplicate
13423	79 Glucose	28 Malic acid	64	0.182	0.442	27.741	0.511	30	112	39	103	59	66 duplicate
8044	79 Glucose	133 [855; Squalene]	64	0.179	0.214	32.348	0.375	31	111	67	75	78	133 original
12248	79 Glucose	18 [590; 1-Acetyl-2-thiohydantoin]	64	0.171	0.401	29.918	0.422	32	110	46	96	68	118 duplicate
14291	79 Glucose	36 [596; N-Acetylglutamic acid (2TMS)]	64	0.158	0.020	12.404	0.541	33	109	81	61	13	50 duplicate
8028	79 Glucose	117 [724; Glyceral (3TMS)]	56	0.155	0.401	34.165	0.497	34	108	47	95	83	73 original
13196	79 Glucose	26 Citramalic acid	64	0.152	0.394	20.081	0.445	35	107	48	94	32	103 duplicate
10435	79 Glucose	4 Phosphoric acid	51	0.151	0.033	9.203	0.459	36	106	79	63	7	95 duplicate
8007	79 Glucose	96 myo-Inositol	49	0.151	0.123	45.210	0.324	37	105	72	70	130	141 original
12611	79 Glucose	21 [876; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	0.145	0.380	20.114	0.475	38	104	50	92	33	85 duplicate
8049	79 Glucose	138 [674; Ergosterol (1TMS)]	46	0.138	0.193	40.209	0.358	39	103	69	73	115	137 original
11750	79 Glucose	14 Fumaric acid	64	0.132	0.432	39.064	0.508	40	102	41	101	112	67 duplicate
14498	79 Glucose	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.131	0.447	30.191	0.533	41	101	37	105	69	56 duplicate
16743	79 Glucose	62 [812; D-Xylofuranose (4TMS)]	64	0.129	0.639	22.172	0.544	42	100	21	121	37	48 duplicate
11105	79 Glucose	9 Proline	63	0.125	-0.090	21.736	0.462	43	99	90	52	36	92 duplicate
10840	79 Glucose	7 Threonine	64	0.124	-0.042	10.033	0.422	44	98	88	56	10	120 duplicate
18254	79 Glucose	56 [829; Orotic acid (3TMS)]	64	0.119	0.621	36.844	0.621	45	97	22	120	104	11 duplicate
15288	79 Glucose	46 Arabinose	64	0.117	0.650	28.649	0.616	46	95	20	122	55	16 duplicate
7999	79 Glucose	88 Gluconic acid	64	0.111	0.517	27.799	0.642	48	94	28	113	60	5 original
17613	79 Glucose	74 [912; Tetradecanoic acid (1TMS)]	64	0.110	0.313	35.854	0.422	49	92	52	90	100	119 duplicate
8012	79 Glucose	101 [832; Dopamine (4TMS)]	64	0.110	0.301	31.958	0.505	50	93	53	89	75	69 original
8002	79 Glucose	81 [766; beta-D-Methylglucopyranoside (4TMS)]	64	0.104	0.252	33.378	0.535	51	91	61	81	83	55 original
13310	79 Glucose	137 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	0.103	-0.178	43.339	0.450	52	90	96	46	126	101 duplicate
8047	79 Glucose	26 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.103	0.092	18.222	0.380	53	89	76	66	28	132 original
12965	79 Glucose	24 [725; 2-Keibocanoic acid (2TMS)]	64	0.096	0.521	8.548	0.631	54	88	28	114	3	7 duplicate
8013	79 Glucose	102 [904; Galactose methoxamine (5TMS)]	64	0.093	0.285	35.950	0.430	55	86	55	87	101	113 original
8011	79 Glucose	100 [857; Mannitol (6TMS)]	64	0.089	0.242	28.608	0.446	56	87	64	78	63	102 original
13081	79 Glucose	25 [709; 2,5-Diaminvalerolactam (2TMS)]	48	0.089	0.022	38.790	0.560	57	85	80	62	111	44 duplicate
11366	79 Glucose	11 Succinic acid	64	0.088	0.492	29.715	0.508	58	84	31	111	67	68 duplicate
8045	79 Glucose	134 Isomaltose	64	0.088	0.588	17.419	0.616	59	83	24	118	24	17 original
12125	79 Glucose	17 [700; 2-methyl-1,2-propanediol (2TMS)]	64	0.083	0.521	20.042	0.539	60	82	27	115	31	52 duplicate
11623	79 Glucose	13 Uracil	64	0.080	0.477	22.237	0.592	61	81	33	109	38	29 duplicate
8014	79 Glucose	103 [648; Ethylamine (2TMS)]	63	0.079	0.344	30.865	0.546	62	80	51	91	74	47 original
14600	79 Glucose	39 [829; 1-Phenylethanol (1TMS)]	63	0.078	0.446	25.879	0.532	63	79	38	104	63	57 duplicate
12001	79 Glucose	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	64	0.076	0.467	19.340	0.592	64	78	35	107	29	30 duplicate
8021	79 Glucose	110 [715; Erythritol (4TMS)]	54	0.075	0.441	37.514	0.643	65	77	40	102	108	4 original
16974	79 Glucose	65 [646; 3-Deoxyglucitol (5TMS)]	63	0.071	0.585	38.968	0.814	66	76	25	117	106	20 duplicate
8022	79 Glucose	111 [583; Erythritol (4TMS)]	42	0.071	0.254	45.500	0.365	67	75	59	83	132	135 original
13535	79 Glucose	29 Erythritol	64	0.067	0.403	33.827	0.512	68	74	44	98	88	65 duplicate
8031	79 Glucose	120 [945; Uridine (3TMS)]	55	0.053	-0.032	23.440	0.416	69	73	85	57	45	122 duplicate
8027	79 Glucose	116 [882; Pseudouridine (5TMS)]	54	0.044	0.159	23.585	0.491	70	72	71	71	46	78 original
13756	79 Glucose	31 [622; Parabanic acid (2TMS)]	64	0.036	-0.113	26.940	0.437	71	71	91	51	56	111 original
12848	79 Glucose	23 Homoserine	64	0.033	-0.253	33.117	0.477	73	69	106	36	80	106 duplicate
8023	79 Glucose	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.033	0.243	47.032	0.438	74	68	63	79	135	83 duplicate
8009	79 Glucose	98 [697; Ribose-5-phosphate methoxamine (5TMS)]	48	0.016	-0.217	44.445	0.438	75	67	100	42	129	110 original
7896	79 Glucose	85 [528; Methylcitric acid (4TMS)]	48	0.009	0.241	29.331	0.452	76	66	65	77	68	109 original
15656	79 Glucose	50 [746; Ribonic acid-1,4-lactone (3TMS)]	61	0.008	0.380	48.900	0.504	77	65	49	93	137	71 duplicate
13665	79 Glucose	32 [728; N,N-Dimethyllysine methyl ester]	63	0.005	-0.225	42.556	0.491	78	64	101	41	123	77 duplicate
8033	79 Glucose	122 [644; Erythritol (4TMS)]	52	-0.002	0.265	43.189	0.585	79	63	57	85	124	31 original

8040	79 Glucose	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	-0.010	0.478	33.904	0.592	80	62	32	110	89	28 original	
8043	79 Glucose	132	[895; Isomaltose methoxyamine (8TMS)]	42	-0.015	0.293	38.559	0.519	81	61	54	88	110	60 original	
8020	79 Glucose	109	Octadecanoic acid	64	-0.016	0.253	20.647	0.452	82	60	82	34	99 original		
12730	79 Glucose	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	-0.017	0.263	39.699	0.530	83	59	58	84	114	58 duplicate	
15095	79 Glucose	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	-0.019	0.234	30.687	0.593	84	58	66	76	73	27 duplicate	
17409	79 Glucose	71	[731; Erythrose (3TMS)]	64	-0.019	-0.069	24.834	0.465	85	57	88	54	49	88 duplicate	
16503	79 Glucose	59	Ornithine; Arginine	64	-0.024	-0.240	13.129	0.454	86	56	104	38	16	98 duplicate	
		135													
8046	79 Glucose	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	-0.027	0.063	24.518	0.389	87	55	78	64	48	131 original		
14988	79 Glucose	43	[548; Leucine (2TBS)]	60	-0.035	-0.086	30.344	0.476	88	54	89	53	71	84 duplicate	
11485	79 Glucose	12	Glyceric acid	63	-0.055	0.250	41.280	0.460	89	53	62	80	119	94 duplicate	
13973	79 Glucose	33	Methionine	64	-0.058	-0.274	33.403	0.424	90	52	110	32	84	118 duplicate	
14080	79 Glucose	34	Aspartic acid	64	-0.059	-0.234	12.851	0.393	91	50	102	40	14	128 duplicate	
7992	79 Glucose	81	Tyrosine	64	-0.059	-0.512	16.860	0.674	92	51	123	19	22	1 original	
11236	79 Glucose	10	Glycine	64	-0.071	-0.552	22.405	0.618	93	49	126	16	40	15 duplicate	
13646	79 Glucose	30	[815; Ethyl-3(2H)-thiophenone]	64	-0.079	-0.238	16.514	0.391	94	48	103	39	20	130 duplicate	
8051	79 Glucose	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	49	-0.082	-0.126	41.445	0.344	95	47	93	49	120	139 original	
8005	79 Glucose	94	Hexadecanoic acid	64	-0.082	0.117	18.129	0.456	96	46	73	69	27	86 original	
		124	[734; 1-Monocleoylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]												
8035	79 Glucose	126	[559; Erythritol (4TMS)]	59	-0.087	-0.271	52.679	0.394	97	45	109	33	140	127 original	
8037	79 Glucose	45	-0.097	-0.067	33.966	0.630	98	44	87	55	90		8 original		
16584	79 Glucose	60	Glycerol-3-phosphate	64	-0.107	-0.363	17.105	0.560	99	43	115	27	23	43 duplicate	
15380	79 Glucose	47	[NA]	64	-0.109	-0.015	34.212	0.432	100	42	83	59	94	112 duplicate	
10298	79 Glucose	3	Ethanolamine	62	-0.113	-0.579	40.722	0.620	101	41	128	14	118	13 duplicate	
14395	79 Glucose	37	Phenylalanine	64	-0.114	-0.317	15.272	0.483	102	40	112	30	18	80 duplicate	
14900	79 Glucose	42	Glutamic acid	60	-0.118	-0.269	21.465	0.423	103	39	108	34	35	117 duplicate	
8050	79 Glucose	139	[700; Ergosta-5,7-dien-3-ol]	38	-0.118	-0.261	40.242	0.335	104	38	107	35	116	140 original	
17268	79 Glucose	69	Arginine	60	-0.134	-0.387	22.368	0.517	105	37	116	26	39	63 duplicate	
17478	79 Glucose	72	[919; D-Xylopyranose (4TMS)]	63	-0.136	-0.164	37.203	0.344	106	36	95	47	107	138 duplicate	
		[826; beta-[[5-methyl-2-thienyl)methyleneamino-													
17808	79 Glucose	77	benzeneacetic acid methyl ester]	62	-0.139	-0.391	19.522	0.465	107	35	117	25	30	89 duplicate	
8010	79 Glucose	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	-0.161	0.271	33.618	0.527	108	34	56	86	88	59 original	
17123	79 Glucose	67	Citric acid	64	-0.173	-0.423	14.222	0.483	109	33	120	22	17	80 duplicate	
15923	79 Glucose	53	Glycerol-2-phosphate	64	-0.179	-0.253	41.455	0.364	110	32	105	37	121	136 duplicate	
15191	79 Glucose	45	Homocysteine	61	-0.184	-0.374	51.600	0.396	111	31	114	26	139	126 duplicate	
16338	79 Glucose	57	[757; 2-Desoxy-pentose-3-ylose dimethoxyamine (2TMS)]	55	-0.185	0.456	30.205	0.616	112	30	36	106	70	18 duplicate	
8019	79 Glucose	108	Octadecanoic acid	64	-0.187	-0.393	38.881	0.414	113	29	118	24	105	123 original	
8048	79 Glucose	137	Ergosterol	64	-0.201	-0.212	27.196	0.367	114	28	89	43	57	134 original	
5746	79 Glucose	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.216	-0.430	44.119	0.443	115	27	121	21	128	104 duplicate	
8052	79 Glucose	141	Lanosta-8,24-dien-3-beta-ol	61	-0.220	-0.336	43.763	0.392	116	26	113	29	127	129 original	
8003	79 Glucose	92	[680; Glycerol-2-phosphate (4TMS)]	54	-0.234	0.617	33.343	0.568	117	25	23	119	81	41 original	
16010	79 Glucose	54	[NA]	55	-0.238	0.402	39.676	0.618	118	24	45	97	113	14 duplicate	
0571	79 Glucose	5	Leucine	45	-0.238	-0.397	33.347	0.477	119	23	119	23	82	82 duplicate	
15473	79 Glucose	48	Asparagine	64	-0.242	-0.680	35.257	0.611	120	22	132	10	97	22 duplicate	
8042	79 Glucose	131	[626; 5-Methylthioadenosine (3TMS)]	55	-0.269	-0.619	45.323	0.568	121	21	130	12	131	39 original	
8008	79 Glucose	97	[758; beta-D-Methylglucopyranoside (4TMS)]	52	-0.281	0.166	23.880	0.661	122	20	70	72	47	2 original	
6664	79 Glucose	61	[NA]	64	-0.286	-0.583	33.598	0.473	123	19	129	13	85	86 duplicate	
5565	79 Glucose	49	[877; Pyrophosphoric acid (4TMS)]	64	-0.305	-0.522	50.057	0.463	124	18	125	17	138	91 duplicate	
7995	79 Glucose	84	Mannitol	62	-0.320	-0.201	16.224	0.514	125	17	98	44	19	64 original	

7993	79 Glucose	82 Lysine	39 -0.331	-0.790	23.257	0.625	126	16	135	7	43	10 original
8039	79 Glucose	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45 -0.337	-0.123	27.929	0.584	127	15	92	50	61	34 original
16098	79 Glucose	55 [612; 4-Aminobutyric acid (2TBS)]	43 -0.340	-0.901	47.115	0.648	128	14	138	4	136	3 duplicate
8038	79 Glucose	127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	39 -0.344	-0.518	28.587	0.519	129	13	124	18	62	61 original
12491	79 Glucose	20 [618; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31 -0.381	-0.844	34.141	0.597	130	12	137	5	92	25 duplicate
10021	79 Glucose	1 [938; Sulfuric acid (2TMS)]	38 -0.381	-0.150	28.936	0.599	131	11	94	48	64	23 duplicate
8001	79 Glucose	80 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	64 -0.387	-0.500	31.976	0.420	132	10	122	20	76	121 original
8004	79 Glucose	93 [607; Putrescine (4TMS)]	60 -0.389	-0.304	46.102	0.487	133	9	111	31	134	79 original
8018	79 Glucose	107 9-(Z)-Octadecenoic acid	64 -0.391	-0.555	23.308	0.399	134	8	127	15	44	124 original
17196	79 Glucose	68 [570; Hypoxanthine (2TMS)]	50 -0.432	-0.823	27.678	0.442	135	7	136	6	58	105 duplicate
8006	79 Glucose	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	20 -0.438	-0.710	46.080	0.519	136	6	133	9	133	62 original
8030	79 Glucose	119 [931; myo-Inositol-2-phosphate (7TMS)]	64 -0.446	-0.626	32.828	0.455	137	5	131	11	79	97 original
8000	79 Glucose	89 [775; Dopamine (4TMS)]	35 -0.583	-0.940	34.377	0.557	138	4	141	1	85	48 original
8016	79 Glucose	105 [705; 2-Ketoglucuronic acid (5TMS)]	48 -0.589	-0.785	30.374	0.625	139	3	134	8	72	9 original
16821	79 Glucose	63 Glutamine	52 -0.656	-0.923	38.433	0.564	140	2	139	3	109	42 duplicate
15835	79 Glucose	52 [NA]	46 -0.697	-0.940	43.193	0.634	141	1	140	2	125	6 duplicate
8059	80 [772; D-Glucose (5TMS)]	87 [945; beta-D-Glucopyranose (5TMS)]	60 0.718	0.960	6.117	0.587	1	141	1	141	1	1 original
8090	80 [772; D-Glucose (5TMS)]	118 [928; Glucopyranose-6-phosphate (6TMS)]	56 0.604	0.789	29.950	0.500	2	140	3	139	88	32 original
14802	80 [772; D-Glucose (5TMS)]	41 [639; Proline (2TMS)]	62 0.414	0.634	19.143	0.471	3	139	19	123	32	47 duplicate
12371	80 [772; D-Glucose (5TMS)]	19 Alanine (BP) (3TMS)	62 0.405	0.718	21.016	0.494	4	138	9	133	41	35 duplicate
15381	80 [772; D-Glucose (5TMS)]	101 [832; Dopamine (4TMS)]	62 0.379	0.528	26.700	0.414	5	137	36	106	74	74 original
17934	80 [772; D-Glucose (5TMS)]	47 [NA]	62 0.370	0.542	27.680	0.397	6	136	34	108	75	87 duplicate
8078	80 [772; D-Glucose (5TMS)]	79 Glucose	62 0.366	0.746	9.477	0.494	7	135	7	135	3	39 duplicate
8075	80 [772; D-Glucose (5TMS)]	106 [733; Threitol (4TMS)]	60 0.336	0.864	24.884	0.489	8	134	16	126	62	38 original
11624	80 [772; D-Glucose (5TMS)]	103 [648; Ethylamine (2TMS)]	61 0.328	0.509	25.851	0.432	9	133	41	101	68	61 original
10707	80 [772; D-Glucose (5TMS)]	6 Glycerol	62 0.325	0.597	18.086	0.477	10	132	27	115	30	44 duplicate
17479	80 [772; D-Glucose (5TMS)]	72 [918; D-Xylopyranose (4TMS)]	62 0.314	0.752	15.605	0.511	11	131	5	137	18	24 duplicate
17340	80 [772; D-Glucose (5TMS)]	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	61 0.313	0.296	31.717	0.329	12	130	59	83	100	129 duplicate
12126	80 [772; D-Glucose (5TMS)]	17 [700; 2-methyl-1,2-propanediol (2TMS)]	55 0.310	0.566	13.833	0.464	13	129	30	112	11	51 duplicate
8095	80 [772; D-Glucose (5TMS)]	123 [945; Galactoturanose-6-phosphate (7TMS)]	62 0.301	0.585	16.405	0.444	14	128	28	114	22	57 duplicate
8063	80 [772; D-Glucose (5TMS)]	91 [766; beta-D-Methylglucopyranoside (4TMS)]	62 0.299	0.615	22.043	0.471	15	127	24	118	49	48 original
8076	80 [772; D-Glucose (5TMS)]	104 [795; Erythritol (4TMS)]	62 0.297	0.460	27.729	0.409	16	126	47	95	78	80 original
8058	80 [772; D-Glucose (5TMS)]	86 [793; D-Galactono-1,4-lactone (4TMS)]	61 0.295	0.528	28.167	0.454	17	125	35	107	79	54 original
15287	80 [772; D-Glucose (5TMS)]	46 Arabinose	59 0.290	0.740	20.045	0.501	18	124	8	134	37	31 original
16875	80 [772; D-Glucose (5TMS)]	65 [646; 3-Deoxyglucitol (5TMS)]	62 0.290	0.707	21.650	0.508	19	123	11	131	46	28 duplicate
11877	80 [772; D-Glucose (5TMS)]	15 Alanine	61 0.287	0.649	31.787	0.538	20	122	17	125	102	12 duplicate
16255	80 [772; D-Glucose (5TMS)]	56 [829; Orolic acid (3TMS)]	62 0.287	0.623	15.186	0.499	21	121	21	121	15	33 duplicate
8106	80 [772; D-Glucose (5TMS)]	134 Isomaltose	62 0.281	0.681	31.714	0.521	22	119	14	128	99	18 duplicate
8060	80 [772; D-Glucose (5TMS)]	88 Glucuronic acid	62 0.281	0.673	13.431	0.511	23	120	15	127	9	23 original
15657	80 [772; D-Glucose (5TMS)]	748; Ribonic acid-1,4-lactone (3TMS)]	62 0.267	0.583	23.261	0.462	24	118	29	113	54	63 original
16744	80 [772; D-Glucose (5TMS)]	62 [812; D-Xylofuranose (4TMS)]	59 0.265	0.562	43.735	0.424	25	117	31	111	137	63 duplicate
17547	80 [772; D-Glucose (5TMS)]	73 [708; Glucose methoxyamine (5TMS)]	62 0.263	0.648	18.659	0.468	26	116	18	124	31	49 duplicate
12866	80 [772; D-Glucose (5TMS)]	24 [725; 2-Ketooctanoic acid (2TMS)]	55 0.262	0.545	30.187	0.422	27	115	33	109	94	67 duplicate
12002	80 [772; D-Glucose (5TMS)]	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	62 0.261	0.607	9.853	0.514	28	114	25	117	4	19 duplicate
8097	80 [772; D-Glucose (5TMS)]	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	62 0.260	0.547	16.007	0.477	29	113	32	110	21	45 duplicate
14601	80 [772; D-Glucose (5TMS)]	39 [829; 1-Phenylethanol (1TMS)]	62 0.258	0.809	7.325	0.509	30	112	2	140	2	27 original
8086	80 [772; D-Glucose (5TMS)]	114 Fructose-6-phosphate	61 0.251	0.527	21.579	0.435	31	111	37	105	45	60 duplicate
13187	80 [772; D-Glucose (5TMS)]	28 Citramalic acid	51 0.242	0.633	29.355	0.510	32	110	20	122	85	26 original
17872	80 [772; D-Glucose (5TMS)]	78 Mannose	60 0.226	0.444	17.327	0.405	33	109	54	88	28	84 duplicate
				0.621	32.040	0.445	34	108	22	120	104	56 duplicate

17745	80 [772; D-Glucose (5TMS; 76 Fructose	62	0,224	0,746	10,345	0,510	35	107	6	136	6	25-tuplicate
8087	80 [772; D-Glucose (5TMS; 115 Glucose-6-phosphate	60	0,211	0,685	9,960	0,513	36	108	12	130	5	20 original
8101	80 [772; D-Glucose (5TMS; 129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	57	0,209	0,616	28,593	0,532	37	105	23	119	81	13 original
8089	80 [772; D-Glucose (5TMS; 117 [724; Glycerol (3TMS)]	54	0,209	0,454	29,562	0,451	38	104	48	94	87	55 original
12731	80 [772; D-Glucose (5TMS; 22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	50	0,208	0,447	34,565	0,417	39	103	51	91	110	70-tuplicate
14499	80 [772; D-Glucose (5TMS; 38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	62	0,205	0,506	25,978	0,415	40	102	42	100	69	72-tuplicate
11751	80 [772; D-Glucose (5TMS; 14 Fumaric acid	62	0,203	0,481	34,385	0,415	41	101	44	98	109	73-tuplicate
11367	80 [772; D-Glucose (5TMS; 11 Succinic acid	62	0,197	0,485	25,622	0,424	42	100	43	99	68	64-tuplicate
14187	80 [772; D-Glucose (5TMS; 35 Pyroglutamic acid	62	0,196	0,715	15,079	0,512	43	99	10	132	14	22-tuplicate
14702	80 [772; D-Glucose (5TMS; 40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	62	0,193	0,448	12,590	0,405	44	98	50	92	8	83-tuplicate
8085	80 [772; D-Glucose (5TMS; 113 Galactose-6-phosphate	60	0,193	0,682	31,158	0,531	45	97	13	129	97	14 original
12612	80 [772; D-Glucose (5TMS; 21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	62	0,193	0,403	17,215	0,380	46	96	56	86	26	99-tuplicate
13424	80 [772; D-Glucose (5TMS; 28 Malic acid	62	0,176	0,465	23,851	0,422	47	95	45	97	58	65-tuplicate
13536	80 [772; D-Glucose (5TMS; 29 Erythritol	62	0,173	0,446	29,499	0,416	48	94	52	90	88	71-tuplicate
8093	80 [772; D-Glucose (5TMS; 121 [657; Erythritol (4TMS)]	53	0,171	0,452	37,733	0,474	49	93	49	93	122	46 original
8088	80 [772; D-Glucose (5TMS; 96 myo-Inositol	47	0,158	0,118	39,890	0,298	50	92	70	72	128	136 original
8084	80 [772; D-Glucose (5TMS; 92 [680; Glycerol-2-phosphate (4TMS)]	52	0,145	0,765	28,628	0,527	51	91	4	138	82	16 original
16011	80 [772; D-Glucose (5TMS; 54 [NA]	53	0,136	0,511	35,662	0,503	52	90	39	103	113	29-tuplicate
12249	80 [772; D-Glucose (5TMS; 18 [590; 1-Acetyl-2-thiohydantoin	62	0,135	0,307	26,075	0,359	53	89	58	84	71	116-tuplicate
16899	80 [772; D-Glucose (5TMS; 64 [788; Tyramine (3TMS)]	61	0,130	0,293	29,959	0,374	54	88	60	82	89	106-tuplicate
16339	80 [772; D-Glucose (5TMS; 57 [757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	53	0,125	0,597	26,016	0,549	55	87	26	116	70	5-tuplicate
8082	80 [772; D-Glucose (5TMS; 110 [715; Erythritol (4TMS)]	52	0,104	0,511	33,286	0,539	56	86	40	102	108	10 original
8089	80 [772; D-Glucose (5TMS; 97 [756; beta-D-Methylglucopyranoside (4TMS)]	50	0,099	0,514	19,181	0,543	57	85	38	104	33	7 original
8099	80 [772; D-Glucose (5TMS; 127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	37	0,090	0,261	24,724	0,523	58	84	63	79	60	17 original
8092	80 [772; D-Glucose (5TMS; 120 [945; Uridine (3TMS)]	52	0,083	0,137	20,437	0,407	59	83	68	74	38	81 original
10022	80 [772; D-Glucose (5TMS; 1 [938; Sulfuric acid (2TMS)]	34	0,080	0,446	25,126	0,558	60	82	53	89	64	3-tuplicate
16422	80 [772; D-Glucose (5TMS; 58 [636; 4R-Acetalamido-2,3-(2-epoxy-4-(E)-hydroxycyclohexane	62	0,065	-0,100	20,950	0,307	62	80	87	55	40	135-tuplicate
10436	80 [772; D-Glucose (5TMS; 4 Phosphoric acid	49	0,065	-0,071	14,886	0,284	63	79	83	59	13	138-tuplicate
11496	80 [772; D-Glucose (5TMS; 12 Glycic acid	61	0,058	0,292	36,720	0,422	64	78	61	81	118	66-tuplicate
17614	80 [772; D-Glucose (5TMS; 74 [912; Tetradecanoic acid (1TMS)]	62	0,053	0,247	31,757	0,384	65	77	64	78	101	98-tuplicate
8071	80 [772; D-Glucose (5TMS; 99 [682; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	39	0,053	0,460	30,063	0,501	66	76	46	96	91	30 original
8072	80 [772; D-Glucose (5TMS; 100 [857; Mannitol (6TMS)]	62	0,052	0,133	25,016	0,378	67	75	69	73	63	103 original
8104	80 [772; D-Glucose (5TMS; 132 [895; Isomaltose methoxyamine (8TMS)]	40	0,049	0,416	35,102	0,484	68	74	55	87	111	42 original
8088	80 [772; D-Glucose (5TMS; 116 [862; Pseudouridine (5TMS)]	28	0,037	-0,162	23,032	0,248	69	73	92	50	53	141 original
8084	80 [772; D-Glucose (5TMS; 122 [844; Erythritol (4TMS)]	50	0,035	0,371	39,229	0,480	70	72	57	85	124	43 original
8094	80 [772; D-Glucose (5TMS; 112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	61	0,025	0,201	42,051	0,373	71	71	65	77	135	107 original
8105	80 [772; D-Glucose (5TMS; 133 [855; Squalene]	62	0,009	0,009	28,785	0,336	72	70	76	66	83	125 original
8055	80 [772; D-Glucose (5TMS; 83 Sorbitol	56	0,001	-0,095	16,918	0,292	73	69	86	56	24	137 original
8057	80 [772; D-Glucose (5TMS; 85 [529; Methylethyl acid (4TMS)]	48	0,001	0,156	24,050	0,349	74	68	66	76	59	120 original
8111	80 [772; D-Glucose (5TMS; 139 [700; Ergosta-5,7-dien-3-ol]	36	0,000	-0,122	35,200	0,276	75	67	89	53	112	140 original
8100	80 [772; D-Glucose (5TMS; 128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	43	-0,012	0,150	24,772	0,541	76	66	67	75	61	8 original
8102	80 [772; D-Glucose (5TMS; 130 Trehalose	61	-0,014	-0,001	12,404	0,329	77	65	78	64	7	130 original
8108	80 [772; D-Glucose (5TMS; 136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	16	-0,017	-0,114	15,697	0,462	78	64	88	54	19	52 original
14999	80 [772; D-Glucose (5TMS; 43 [548; Leucine (2TBS)]	59	-0,027	-0,127	26,628	0,385	79	63	90	52	73	93-tuplicate
13082	80 [772; D-Glucose (5TMS; 25 [709; 2,5-Diaminohexanoic acid (2TMS)]	47	-0,029	-0,286	36,469	0,486	80	62	96	46	117	41-tuplicate
8077	80 [772; D-Glucose (5TMS; 105 [705; 2-Ketoglucuronic acid (5TMS)]	46	-0,043	-0,008	26,618	0,562	81	61	80	62	72	2 original
8074	80 [772; D-Glucose (5TMS; 102 [904; Galactose methoxyamine (5TMS)]	62	-0,046	0,047	31,837	0,382	82	60	74	68	103	97 original
8112	80 [772; D-Glucose (5TMS; 140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	47	-0,047	-0,090	36,265	0,317	83	59	84	58	116	134 original

15096	80 [772; D-Glucose (5TMS); 44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	48	-0.055	0.066	28.237	0.547	84	58	73	69	80	6 duplicate
17680	80 [772; D-Glucose (5TMS); 75	Lysine	62	-0.069	-0.210	17.684	0.338	85	57	93	49	29	124 duplicate
8107	80 [772; D-Glucose (5TMS); 135	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	62	-0.071	0.015	21.289	0.360	86	56	75	67	42	115 original
8110	80 [772; D-Glucose (5TMS); 138	[674; Ergosterol (1TMS)]	44	-0.074	0.002	36.104	0.372	87	55	77	65	115	109 original
13311	80 [772; D-Glucose (5TMS); 27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	51	-0.098	-0.373	39.433	0.369	88	54	105	37	126	89 duplicate
8056	80 [772; D-Glucose (5TMS); 84	Mannitol	61	-0.109	0.111	15.940	0.368	89	53	71	20	92	original
15924	80 [772; D-Glucose (5TMS); 53	Glycerol-2-phosphate	62	-0.112	-0.048	36.814	0.394	90	52	81	61	119	88 duplicate
14292	80 [772; D-Glucose (5TMS); 36	[596; N-Acetylglutamic acid (2TMS)]	62	-0.132	-0.281	15.446	0.365	91	51	95	47	16	111 duplicate
8098	80 [772; D-Glucose (5TMS); 126	[559; Erythritol (4TMS)]	43	-0.150	-0.092	30.904	0.552	92	50	85	57	96	4 original
8081	80 [772; D-Glucose (5TMS); 109	Octadecanoic acid	62	-0.152	0.101	19.704	0.404	93	49	72	70	36	88 original
10161	80 [772; D-Glucose (5TMS); 2	Serine	60	-0.164	-0.297	25.711	0.334	94	48	97	45	67	127 duplicate
8065	80 [772; D-Glucose (5TMS); 93	[607; Putrescine (4TMS)]	58	-0.175	-0.067	40.823	0.385	95	47	82	60	130	95 original
8083	80 [772; D-Glucose (5TMS); 111	[583; Erythritol (4TMS)]	40	-0.177	-0.139	40.968	0.379	96	46	91	51	131	101 original
8066	80 [772; D-Glucose (5TMS); 94	Hexadecanoic acid	62	-0.184	-0.005	17.318	0.410	97	45	79	63	27	77 original
8113	80 [772; D-Glucose (5TMS); 141	Lanosta-8,24-dien-3-beta-ol	59	-0.184	-0.278	38.701	0.321	98	44	94	48	123	133 original
17050	80 [772; D-Glucose (5TMS); 66	Glyceral acid-3-phosphate	62	-0.195	-0.340	32.175	0.356	99	43	100	42	105	119 duplicate
8070	80 [772; D-Glucose (5TMS); 98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	47	-0.219	-0.437	41.249	0.365	100	42	110	32	132	94 original
8062	80 [772; D-Glucose (5TMS); 90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	62	-0.222	-0.357	28.115	0.362	101	41	102	40	78	113 original
15566	80 [772; D-Glucose (5TMS); 49	[877; Pyrophosphoric acid (4TMS)]	62	-0.240	-0.440	45.144	0.377	102	40	112	30	138	104 duplicate
12849	80 [772; D-Glucose (5TMS); 23	Homoserine	62	-0.251	-0.452	30.126	0.429	103	39	113	29	93	62 duplicate
8109	80 [772; D-Glucose (5TMS); 137	Ergosterol	62	-0.266	-0.367	25.255	0.328	104	38	104	38	65	132 original
15192	80 [772; D-Glucose (5TMS); 45	Homocysteine	59	-0.268	-0.477	46.488	0.387	105	37	118	24	139	91 duplicate
8096	80 [772; D-Glucose (5TMS); 124	[734; 1-Monoleoylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	57	-0.269	-0.332	49.472	0.332	106	36	99	43	140	128 original
11106	80 [772; D-Glucose (5TMS); 9	Proline	61	-0.272	-0.358	23.752	0.335	107	35	103	39	56	126 duplicate
17410	80 [772; D-Glucose (5TMS); 71	[731; Erythrose (3TMS)]	62	-0.274	-0.344	21.966	0.373	108	34	101	41	48	108 duplicate
13866	80 [772; D-Glucose (5TMS); 32	[729; N,N-Dimethyllysine methyl ester]	61	-0.282	-0.454	39.246	0.420	109	33	114	28	125	68 duplicate
10841	80 [772; D-Glucose (5TMS); 7	Threonine	62	-0.297	-0.383	13.754	0.328	110	32	107	35	10	131 duplicate
13757	80 [772; D-Glucose (5TMS); 31	[622; Parabanic acid (2TMS)]	62	-0.301	-0.476	36.842	0.380	111	31	117	25	120	100 duplicate
14081	80 [772; D-Glucose (5TMS); 34	Aspartic acid	62	-0.307	-0.378	16.909	0.357	112	30	106	36	23	118 duplicate
10974	80 [772; D-Glucose (5TMS); 8	Isoleucine	53	-0.331	-0.299	22.832	0.277	113	29	98	44	52	139 duplicate
8079	80 [772; D-Glucose (5TMS); 107	9-(Z)-Octadecenoic acid	62	-0.338	-0.502	20.750	0.366	114	28	120	22	39	110 original
16504	80 [772; D-Glucose (5TMS); 59	Ornithine; Arginine	62	-0.344	-0.472	19.636	0.364	115	27	115	27	35	112 duplicate
8080	80 [772; D-Glucose (5TMS); 108	Octadecenoic acid	62	-0.353	-0.438	32.829	0.362	116	26	111	31	107	114 original
17269	80 [772; D-Glucose (5TMS); 69	Arginine	58	-0.376	-0.539	22.168	0.441	117	25	122	20	50	58 duplicate
13974	80 [772; D-Glucose (5TMS); 33	Methionine	62	-0.379	-0.421	30.279	0.381	118	24	109	33	95	98 duplicate
8103	80 [772; D-Glucose (5TMS); 131	[626; 5-Methylthioadenosine (3TMS)]	54	-0.385	-0.610	41.495	0.540	119	23	125	17	133	9 original
8091	80 [772; D-Glucose (5TMS); 119	[931; myo-Inositol-2-phosphate (7TMS)]	62	-0.390	-0.506	29.208	0.388	120	22	121	21	84	90 original
16585	80 [772; D-Glucose (5TMS); 60	Glycerol-3-phosphate	62	-0.395	-0.600	16.941	0.413	121	21	124	18	25	75 duplicate
13647	80 [772; D-Glucose (5TMS); 30	[815; Ethyl-3(2H)-thiophenone]	62	-0.411	-0.418	19.345	0.346	122	20	108	34	34	122 duplicate
16822	80 [772; D-Glucose (5TMS); 63	Glutamine	50	-0.422	-0.796	35.770	0.488	123	19	138	4	114	40 duplicate
8054	80 [772; D-Glucose (5TMS); 82	Lysine	37	-0.429	-0.726	21.429	0.494	124	18	131	11	43	37 original
14901	80 [772; D-Glucose (5TMS); 42	Glutamic acid	58	-0.445	-0.473	23.815	0.379	125	17	116	26	57	102 duplicate
12492	80 [772; D-Glucose (5TMS); 20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.445	-0.733	30.078	0.406	126	16	133	9	92	82 duplicate
8067	80 [772; D-Glucose (5TMS); 95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	49	-0.456	-0.674	42.390	0.409	127	15	129	13	136	78 original
17809	80 [772; D-Glucose (5TMS); 77	[826; beta-[(5-methyl-2-thienyl)methyleneamino]-benzeneacetic acid methyl ester]	60	-0.459	-0.599	22.660	0.375	128	14	123	19	51	105 duplicate
8053	80 [772; D-Glucose (5TMS); 81	Tyrosine	62	-0.460	-0.711	21.520	0.528	129	13	130	12	44	16 original
11237	80 [772; D-Glucose (5TMS); 10	Glycine	62	-0.480	-0.728	21.913	0.512	130	12	132	10	47	21 duplicate

15474	80 [772; D-Glucose (5TMS)	48 Asparagine	62 -0.482	-0.759	32.642	0.497	131	11	135	7	108	34 duplicate
14396	80 [772; D-Glucose (5TMS)	37 Phenylalanine	62 -0.503	-0.828	15.460	0.412	132	10	128	16	17	76 duplicate
15836	80 [772; D-Glucose (5TMS)	52 [NA]	45 -0.517	-0.756	39.535	0.439	133	9	134	8	127	59 duplicate
16097	80 [772; D-Glucose (5TMS)	55 [612; 4-Aminobutyric acid (2TBS)]	42 -0.519	-0.838	41.827	0.466	134	8	139	3	134	50 duplicate
10299	80 [772; D-Glucose (5TMS)	3 Ethanolamine	60 -0.529	-0.783	37.219	0.539	135	7	137	5	121	11 duplicate
10572	80 [772; D-Glucose (5TMS)	5 Leucine	43 -0.530	-0.482	27.924	0.342	136	6	119	23	77	123 duplicate
17124	80 [772; D-Glucose (5TMS)	67 Citric acid	62 -0.541	-0.870	14.560	0.409	137	5	128	14	12	79 duplicate
16665	80 [772; D-Glucose (5TMS)	61 [NA]	62 -0.542	-0.770	30.042	0.492	138	4	136	6	90	38 duplicate
15747	80 [772; D-Glucose (5TMS)	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44 -0.562	-0.632	40.208	0.404	139	3	127	15	129	85 duplicate
8081	80 [772; D-Glucose (5TMS)	775; Dopamine (4TMS)]	34 -0.597	-0.848	31.480	0.417	140	2	140	2	88	89 original
17197	80 [772; D-Glucose (5TMS)	68 [570; Hypoxanthine (2TMS)]	19 -0.719	-0.855	23.460	0.347	141	1	141	1	55	121 duplicate
17810	81 Tyrosine	[826; beta-[[5-methyl-2-thienyl)methyl]eneamino-benzeneacetic acid methyl ester]	62 0.847	0.933	7.560	0.591	1	141	4	138	2	58 duplicate
8114	81 Tyrosine	82 Lysine	39 0.806	0.946	19.636	0.699	2	140	1	141	26	4 original
14902	81 Tyrosine	42 Glutamic acid	60 0.800	0.860	11.476	0.550	3	139	13	129	10	75 duplicate
10300	81 Tyrosine	3 Ethanolamine	62 0.797	0.943	37.318	0.682	4	138	2	140	107	11 duplicate
11238	81 Tyrosine	10 Glycine	64 0.781	0.903	16.198	0.658	5	137	6	136	19	22 duplicate
16098	81 Tyrosine	55 [612; 4-Aminobutyric acid (2TBS)]	43 0.772	0.941	48.027	0.696	6	136	3	139	138	6 duplicate
15748	81 Tyrosine	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44 0.748	0.829	45.629	0.596	7	135	15	127	133	52 duplicate
17270	81 Tyrosine	69 Arginine	60 0.747	0.868	15.615	0.594	8	134	10	132	17	56 duplicate
16505	81 Tyrosine	59 Ornithine; Arginine	64 0.743	0.830	10.705	0.526	9	133	14	128	8	83 duplicate
14397	81 Tyrosine	37 Phenylalanine	64 0.720	0.886	13.089	0.568	10	132	8	134	13	68 duplicate
13648	81 Tyrosine	30 [815; Ethyl-3-(2H)-thiophenone]	64 0.713	0.756	8.873	0.496	11	131	20	122	4	104 duplicate
17125	81 Tyrosine	67 Citric acid	64 0.691	0.878	12.726	0.535	12	130	9	133	12	87 duplicate
17188	81 Tyrosine	68 [570; Hypoxanthine (2TMS)]	20 0.684	0.888	33.287	0.571	13	129	7	135	85	67 duplicate
13867	81 Tyrosine	32 [728; N,N-Dimethyllysine methyl ester]	63 0.683	0.867	38.009	0.610	14	128	11	131	111	42 duplicate
10573	81 Tyrosine	5 Leucine	45 0.679	0.694	34.238	0.597	15	127	28	114	92	50 duplicate
15475	81 Tyrosine	48 Asparagine	64 0.654	0.803	28.744	0.636	16	125	16	126	66	29 duplicate
13975	81 Tyrosine	33 Methionine	64 0.654	0.698	29.588	0.467	17	126	27	115	64	115 duplicate
16586	81 Tyrosine	60 Glycerol-3-phosphate	64 0.652	0.860	13.853	0.596	18	124	12	130	15	54 duplicate
11107	81 Tyrosine	9 Proline	63 0.621	0.793	13.869	0.519	19	123	17	125	16	98 duplicate
10975	81 Tyrosine	8 Isoleucine	55 0.576	0.693	20.749	0.461	20	122	29	113	31	119 duplicate
8121	81 Tyrosine	89 [775; Dopamine (4TMS)]	35 0.573	0.770	34.108	0.670	21	121	18	124	89	14 original
8127	81 Tyrosine	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50 0.572	0.840	44.933	0.573	22	120	35	107	132	68 original
14082	81 Tyrosine	34 Aspartic acid	64 0.569	0.655	8.265	0.444	23	119	34	108	3	123 duplicate
13758	81 Tyrosine	31 [622; Parabanic acid (2TMS)]	64 0.566	0.739	38.347	0.500	24	118	21	121	112	102 duplicate
17051	81 Tyrosine	66 Glycine acid-3-phosphate	64 0.527	0.758	34.181	0.528	25	117	19	123	90	91 duplicate
10842	81 Tyrosine	7 Threonine	64 0.518	0.735	9.047	0.506	26	116	22	120	6	101 duplicate
10162	81 Tyrosine	2 Serine	62 0.515	0.731	21.597	0.555	27	115	23	119	36	71 duplicate
12493	81 Tyrosine	20 [819; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	31 0.501	0.920	37.926	0.697	28	114	5	137	108	5 duplicate
8163	81 Tyrosine	131 [626; 5-Methylthioadenosine (3TMS)]	55 0.492	0.509	42.982	0.616	29	113	41	101	130	38 original
15193	81 Tyrosine	45 Homocysteine	61 0.486	0.497	49.908	0.460	30	112	43	99	139	120 duplicate
16666	81 Tyrosine	61 [NA]	64 0.455	0.525	31.521	0.499	31	111	40	102	78	103 duplicate
12850	81 Tyrosine	23 Homoserine	64 0.454	0.716	29.332	0.554	32	110	24	118	63	72 duplicate
8168	81 Tyrosine	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17 0.412	0.491	13.463	0.321	33	109	44	98	14	141 original
8130	81 Tyrosine	98 [697; Ribose-5-phosphate methoxymethylamine (5TMS)]	48 0.408	0.655	42.878	0.553	34	108	33	109	129	74 original
15567	81 Tyrosine	49 [877; Pyrophosphoric acid (4TMS)]	64 0.401	0.404	46.754	0.474	35	107	48	94	135	114 duplicate
13312	81 Tyrosine	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53 0.396	0.708	41.716	0.532	36	106	26	116	126	88 duplicate
17681	81 Tyrosine	75 Lysine	64 0.392	0.673	10.840	0.543	37	105	31	111	9	84 duplicate
14293	81 Tyrosine	36 [596; N-Acetylglutamic acid (2TMS)]	64 0.378	0.711	8.944	0.549	38	104	25	117	5	76 duplicate

17411	81 Tyrosine	71 [731; Erythrose (3TMS)]	64 0.359	0.577	23.574	0.479	39	103	37	105	48	111 duplicate
8140	81 Tyrosine	108 Octadecanoic acid	64 0.357	0.540	34.658	0.442	40	102	39	103	95	124 original
13083	81 Tyrosine	25 [709; 2,5-Diaminovalerolactam (2TMS)]	48 0.307	0.677	30.283	0.595	41	101	30	112	69	55 duplicate
15837	81 Tyrosine	52 [NA]	46 0.299	0.583	40.628	0.704	42	100	38	108	121	1 duplicate
16423	81 Tyrosine	58 [636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64 0.288	0.569	20.544	0.523	43	99	38	104	27	96 duplicate
8156	81 Tyrosine	124 [734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecenoylethanol (1TMS)]	59 0.245	0.464	51.494	0.385	44	98	48	96	140	136 original
8162	81 Tyrosine	130 Trehalose	63 0.222	0.344	10.357	0.428	45	97	50	92	7	128 original
8169	81 Tyrosine	137 Ergosterol	64 0.212	0.418	24.323	0.411	46	96	47	95	50	133 original
15000	81 Tyrosine	43 [548; Leucine (2TBS)]	60 0.190	0.221	29.677	0.508	47	95	53	89	65	100 duplicate
8139	81 Tyrosine	119 [931; myo-Inositol-2-phosphate (7TMS)]	64 0.189	0.318	30.278	0.481	48	94	51	91	68	109 original
8139	81 Tyrosine	107 9-(Z)-Octadecenoic acid	64 0.176	0.364	21.453	0.400	49	93	49	93	33	134 original
16823	81 Tyrosine	63 Glutamine	52 0.169	0.657	33.385	0.625	50	92	32	110	86	33 duplicate
8170	81 Tyrosine	138 [674; Ergosterol (1TMS)]	46 0.161	0.262	40.524	0.476	51	91	52	90	120	113 original
10437	81 Tyrosine	4 Phosphoric acid	51 0.114	0.480	7.176	0.455	52	90	45	97	1	121 duplicate
8171	81 Tyrosine	139 [700; Ergosta-5,7-dien-3-ol]	38 0.098	0.188	40.703	0.368	53	89	55	87	122	138 original
8128	81 Tyrosine	94 Hexadecanoic acid	64 0.095	0.107	18.081	0.583	54	88	57	85	23	62 original
8173	81 Tyrosine	141 Lanosta-8,24-dien-3-beta-ol	61 0.082	0.183	42.584	0.482	55	87	56	88	127	108 original
8141	81 Tyrosine	109 Octadecanoic acid	64 0.074	0.015	21.757	0.545	56	86	59	83	38	82 original
8143	81 Tyrosine	111 [583; Erythritol (4TMS)]	42 0.068	0.004	41.363	0.332	57	85	60	82	125	139 original
16900	81 Tyrosine	64 [789; Tyramine (3TMS)]	63 0.050	-0.190	33.214	0.488	58	84	67	75	83	106 duplicate
8165	81 Tyrosine	133 [855; Squalene]	64 0.033	0.212	31.328	0.415	59	83	54	88	77	132 original
8115	81 Tyrosine	80 Sorbitol	58 0.032	0.501	16.041	0.531	60	82	42	100	18	89 original
8122	81 Tyrosine	90 [910; 9-(Z)-Hexadecanoic acid (1TMS)]	64 -0.011	0.056	30.435	0.464	61	81	58	84	70	118 original
11878	81 Tyrosine	15 Alanine	64 -0.016	-0.354	21.658	0.662	62	80	75	67	37	18 duplicate
17480	81 Tyrosine	72 [919; D-Xylopyranose (4TMS)]	63 -0.017	-0.022	36.177	0.376	63	79	63	78	103	137 duplicate
8172	81 Tyrosine	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49 -0.024	-0.018	42.768	0.422	64	78	62	80	128	130 original
17935	81 Tyrosine	79 Glucose	64 -0.059	-0.512	16.860	0.674	65	77	88	54	20	12 duplicate
8150	81 Tyrosine	118 [928; Glucopyranose-6-phosphate (6TMS)]	58 -0.089	-0.279	34.197	0.438	66	76	70	72	91	125 original
8158	81 Tyrosine	126 [559; Erythritol (4TMS)]	45 -0.091	-0.009	25.567	0.669	67	75	61	81	54	16 original
15925	81 Tyrosine	53 Glycerol-2-phosphate	64 -0.096	-0.121	40.270	0.422	68	74	65	77	119	131 duplicate
8125	81 Tyrosine	123 [945; Galactofuranose-6-phosphate (7TMS)]	64 -0.106	-0.309	28.561	0.652	69	73	72	70	56	25 original
8146	81 Tyrosine	93 [607; Putrescine (4TMS)]	60 -0.118	-0.382	44.836	0.520	70	72	78	64	131	97 original
8148	81 Tyrosine	114 Fructose-6-phosphate	53 -0.120	-0.522	34.830	0.649	71	71	90	52	98	26 original
8116	81 Tyrosine	116 [982; Pseudouridine (5TMS)]	30 -0.136	-0.055	28.803	0.465	72	70	64	78	62	116 original
8116	81 Tyrosine	84 Mannitol	62 -0.139	-0.626	20.642	0.607	73	69	100	42	29	45 original
8167	81 Tyrosine	135 [902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64 -0.145	-0.271	24.129	0.428	74	68	69	73	48	129 original
8128	81 Tyrosine	96 myo-Inositol	49 -0.148	-0.182	46.919	0.329	75	67	68	76	136	140 original
8145	81 Tyrosine	113 Galactose-6-phosphate	62 -0.170	-0.588	37.072	0.660	76	66	95	47	105	21 original
17615	81 Tyrosine	74 [912; Tetradecanoic acid (1TMS)]	64 -0.216	-0.265	36.362	0.545	77	65	68	74	104	79 duplicate
14803	81 Tyrosine	41 [639; Proline (2TMS)]	64 -0.222	-0.308	24.241	0.516	78	64	71	71	49	99 duplicate
8159	81 Tyrosine	127 [777; Fructose-6-phosphate methoxamine (6TMS)]	39 -0.233	-0.386	20.716	0.479	79	63	79	63	30	112 original
8134	81 Tyrosine	102 [904; Galactose methoxamine (5TMS)]	64 -0.237	-0.406	35.528	0.434	80	62	80	62	101	127 original
8136	81 Tyrosine	104 [795; Erythritol (4TMS)]	63 -0.244	-0.313	33.280	0.671	81	61	73	69	84	13 original
12250	81 Tyrosine	18 [590; 1-Acetyl-2-thiohydantoin]	64 -0.245	-0.315	29.919	0.438	82	60	74	68	67	126 duplicate
8164	81 Tyrosine	132 [895; Isomaltose methoxamine (8TMS)]	42 -0.250	-0.678	35.454	0.525	83	59	101	41	100	84 original
8144	81 Tyrosine	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63 -0.261	-0.447	46.214	0.481	84	58	83	59	134	110 original
8117	81 Tyrosine	85 [529; Methylcitric acid (4TMS)]	48 -0.277	-0.422	31.954	0.549	85	57	81	61	80	77 original
12372	81 Tyrosine	19 Alanine (BP) (3TMS)	64 -0.277	-0.474	27.356	0.585	86	58	84	58	59	60 duplicate



15097	81 Tyrosine	44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	50 -0.278	-0.375	25.099	0.645	87	55	77	65	53	28 duplicate
8132	81 Tyrosine	100 [857; Mannitol (6TMS)]	64 -0.299	-0.510	28.782	0.453	88	54	87	55	61	122 original
16382	81 Tyrosine	47 [NA]	64 -0.332	-0.484	34.828	0.524	89	53	85	57	97	95 duplicate
8154	81 Tyrosine	122 [644; Erythritol (4TMS)]	52 -0.354	-0.519	38.453	0.827	90	52	89	53	113	32 original
8153	81 Tyrosine	121 [657; Erythritol (4TMS)]	55 -0.374	-0.444	39.499	0.607	91	51	82	60	117	46 original
14188	81 Tyrosine	35 Pyroglutamic acid	64 -0.379	-0.748	17.528	0.609	92	50	110	32	22	43 duplicate
8152	81 Tyrosine	120 [945; Uridine (3TMS)]	54 -0.381	-0.355	21.848	0.530	93	49	76	66	41	90 original
8149	81 Tyrosine	117 [724; Glycerol (3TMS)]	56 -0.383	-0.507	32.944	0.591	94	48	86	56	81	57 original
8142	81 Tyrosine	110 [715; Erythritol (4TMS)]	54 -0.385	-0.552	34.607	0.703	95	47	91	51	93	3 original
8147	81 Tyrosine	115 Glucose-6-phosphate	62 -0.387	-0.708	18.488	0.599	96	46	105	37	24	49 original
10708	81 Tyrosine	6 Glycerol	64 -0.412	-0.706	17.105	0.633	97	45	104	38	21	30 duplicate
13198	81 Tyrosine	26 Citramalic acid	64 -0.427	-0.594	20.631	0.465	98	44	96	46	28	117 duplicate
8160	81 Tyrosine	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45 -0.438	-0.623	21.826	0.541	100	42	97	45	40	85 original
12613	81 Tyrosine	21 [878; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	64 -0.447	-0.625	21.802	0.483	101	41	99	43	39	107 duplicate
17896	81 Tyrosine	80 [772; D-Glucose (5TMS)]	62 -0.460	-0.711	21.520	0.528	102	40	108	36	35	92 duplicate
14703	81 Tyrosine	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	64 -0.464	-0.624	12.395	0.515	103	39	98	44	11	39 duplicate
13425	81 Tyrosine	28 Malic acid	64 -0.468	-0.737	28.390	0.566	104	38	108	34	60	69 duplicate
8157	81 Tyrosine	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64 -0.483	-0.786	21.135	0.804	105	37	113	29	32	48 original
17548	81 Tyrosine	73 [708; Glucose methoxyamine (5TMS)]	64 -0.485	-0.578	38.008	0.588	106	36	93	49	110	59 duplicate
17746	81 Tyrosine	76 Fructose	64 -0.494	-0.779	23.183	0.613	107	35	112	30	43	40 duplicate
11497	81 Tyrosine	12 Glycic acid	63 -0.494	-0.723	40.758	0.492	108	34	107	35	123	105 duplicate
17873	81 Tyrosine	78 Mannose	62 -0.513	-0.697	39.386	0.546	109	33	103	39	116	78 duplicate
12732	81 Tyrosine	22 [690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	52 -0.514	-0.740	38.873	0.539	110	32	109	33	114	88 duplicate
8138	81 Tyrosine	106 [733; Threitol (4TMS)]	62 -0.517	-0.686	32.947	0.703	111	31	102	40	82	2 original
8123	81 Tyrosine	91 [766; beta-D-Methylglucopyranoside (4TMS)]	64 -0.518	-0.830	37.948	0.608	112	30	119	23	109	44 original
11752	81 Tyrosine	4 Fumaric acid	64 -0.550	-0.778	39.110	0.554	113	29	111	31	115	73 duplicate
10023	81 Tyrosine	1 [938; Sulfuric acid (2TMS)]	36 -0.556	-0.862	23.205	0.623	114	28	127	15	44	35 duplicate
8129	81 Tyrosine	97 [756; beta-D-Methylglucopyranoside (4TMS)]	52 -0.560	-0.923	25.792	0.690	115	27	141	1	55	7 original
8133	81 Tyrosine	101 [832; Dopamine (4TMS)]	64 -0.565	-0.828	34.645	0.611	116	26	118	24	94	41 original
8119	81 Tyrosine	87 [945; beta-D-Glucopyranose (5TMS)]	62 -0.572	-0.794	22.109	0.544	117	25	116	26	42	83 original
11368	81 Tyrosine	11 Succinic acid	64 -0.577	-0.788	30.463	0.545	118	24	114	28	71	81 duplicate
14500	81 Tyrosine	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	64 -0.580	-0.821	31.312	0.580	119	23	117	25	76	63 duplicate
8131	81 Tyrosine	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41 -0.590	-0.835	30.819	0.598	120	22	120	22	73	51 original
17341	81 Tyrosine	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57 -0.591	-0.576	21.462	0.545	121	21	92	50	34	80 duplicate
8135	81 Tyrosine	103 [648; Ethylamine (2TMS)]	63 -0.602	-0.852	34.898	0.624	122	20	124	18	99	34 original
8124	81 Tyrosine	92 [680; Glycerol-2-phosphate (4TMS)]	54 -0.607	-0.792	30.790	0.561	123	19	115	27	72	70 original
8137	81 Tyrosine	105 [705; 2-Ketogluconic acid (5TMS)]	48 -0.613	-0.839	24.483	0.649	124	18	123	19	51	27 original
13537	81 Tyrosine	29 Erythritol	64 -0.614	-0.839	33.967	0.604	125	18	121	21	88	47 duplicate
16745	81 Tyrosine	62 [812; D-Xylofuranose (4TMS)]	64 -0.614	-0.839	24.033	0.576	126	17	122	20	47	64 duplicate
16012	81 Tyrosine	54 [NA]	55 -0.665	-0.881	37.253	0.575	127	15	129	13	106	65 duplicate
8120	81 Tyrosine	88 Gluconic acid	64 -0.684	-0.865	31.523	0.669	128	14	128	14	79	15 original
14602	81 Tyrosine	39 [829; 1-Phenylethanol (1TMS)]	63 -0.689	-0.859	30.971	0.584	129	13	125	17	74	61 duplicate
8118	81 Tyrosine	96 [793; D-Galactono-1,4-lactone (4TMS)]	61 -0.691	-0.899	34.678	0.654	130	12	133	9	96	24 original
12127	81 Tyrosine	17 [700; 2-methyl-1,2-propanediol (2TMS)]	64 -0.691	-0.861	24.651	0.621	131	11	126	16	52	37 duplicate
16256	81 Tyrosine	56 [828; Orotic acid (3TMS)]	64 -0.709	-0.916	40.253	0.668	132	10	137	5	118	17 duplicate
12967	81 Tyrosine	24 [725; 2-Ketotartaric acid (2TMS)]	64 -0.712	-0.907	18.610	0.684	133	9	136	6	25	8 duplicate
12003	81 Tyrosine	16 [844; 2-Methyl-1,3-butanediol (2TMS)]	64 -0.722	-0.898	23.287	0.683	134	8	132	10	45	9 duplicate
16340	81 Tyrosine	57 [757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55 -0.731	-0.894	31.287	0.621	135	7	130	12	75	36 duplicate
8166	81 Tyrosine	134 Isomaltose	64 -0.732	-0.918	27.261	0.681	136	6	139	3	58	19 original

8161	81 Tyrosine	128	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	-0.732	-0.902	35.761	0.633	137	5	135	7	102	31 original
15288	81 Tyrosine	46	Arabinose	64	-0.745	-0.919	33.948	0.661	138	4	140	2	87	20 duplicate
16976	81 Tyrosine	65	[646; 3-Deoxyglucitol (5TMS)]	63	-0.753	-0.900	41.020	0.657	139	3	134	8	124	23 duplicate
15658	81 Tyrosine	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	-0.764	-0.894	47.895	0.596	140	2	131	11	137	53 duplicate
11625	81 Tyrosine	13	Uracil	64	-0.802	-0.918	28.934	0.683	141	1	138	4	57	10 duplicate
17413	83 Sorbitol	71	[731; Erythrose (3TMS)]	58	0.614	0.677	10.958	0.451	1	141	6	136	16	37 duplicate
8263	83 Sorbitol	114	Fructose-6-phosphate	47	0.584	0.161	21.893	0.383	2	140	47	95	87	70 original
8262	83 Sorbitol	113	Galactose-6-phosphate	56	0.569	0.102	23.013	0.404	3	139	56	86	97	63 original
8265	83 Sorbitol	116	[882; Pseudouridine (5TMS)]	30	0.517	0.578	19.508	0.485	4	138	12	130	72	24 original
8234	83 Sorbitol	85	[529; Methylcitric acid (4TMS)]	48	0.498	0.731	18.803	0.541	5	137	2	140	63	6 original
8272	83 Sorbitol	123	[945; Galactoturanose-6-phosphate (7TMS)]	58	0.486	0.301	13.021	0.417	6	136	30	112	29	47 original
17550	83 Sorbitol	73	[708; Glucose methoxyamine (5TMS)]	54	0.459	0.094	23.854	0.416	7	135	59	83	102	48 duplicate
8287	83 Sorbitol	138	[674; Ergosterol (1TMS)]	41	0.439	0.395	27.648	0.372	8	134	24	118	121	80 original
8264	83 Sorbitol	115	Glucose-6-phosphate	56	0.434	-0.002	11.507	0.307	9	133	74	68	19	126 original
8282	83 Sorbitol	133	[855; Squalene]	58	0.425	0.250	17.965	0.390	10	132	37	105	56	63 original
8253	83 Sorbitol	104	[795; Erythritol (4TMS)]	58	0.422	0.270	19.031	0.388	11	131	38	108	66	68 original
14190	83 Sorbitol	35	Pyroglutamic acid	58	0.400	-0.053	22.210	0.325	12	130	81	61	90	117 duplicate
8243	83 Sorbitol	94	Hexadecanoic acid	58	0.389	0.372	9.307	0.341	13	129	27	115	6	106 original
12252	83 Sorbitol	18	[590; 1-Acetyl-2-thiohydantoin]	58	0.388	0.151	16.483	0.319	14	128	50	92	47	121 duplicate
8258	83 Sorbitol	109	Octadecanoic acid	58	0.377	0.386	12.275	0.354	15	127	26	116	24	96 original
12374	83 Sorbitol	102	Alanine (BP) (3TMS)	58	0.364	-0.039	21.959	0.326	17	125	78	64	88	81 duplicate
8251	83 Sorbitol	102	[904; Galactose methoxyamine (5TMS)]	58	0.360	-0.048	15.758	0.321	18	124	79	63	41	119 original
8249	83 Sorbitol	100	[857; Mannitol (6TMS)]	58	0.360	-0.048	15.758	0.321	18	124	79	63	41	119 original
13427	83 Sorbitol	28	Malic acid	58	0.358	-0.156	15.383	0.391	19	123	95	47	40	62 duplicate
10844	83 Sorbitol	7	Theonine	58	0.330	0.598	12.079	0.502	20	122	10	132	23	16 duplicate
8275	83 Sorbitol	126	[559; Erythritol (4TMS)]	39	0.323	0.239	18.399	0.424	21	121	39	103	59	45 original
8284	83 Sorbitol	135	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	58	0.316	0.020	11.972	0.331	22	120	70	72	21	113 original
8270	83 Sorbitol	49	[657; Erythritol (4TMS)]	49	0.316	0.159	27.379	0.312	23	119	49	93	119	124 original
8260	83 Sorbitol	111	[583; Erythritol (4TMS)]	37	0.315	0.085	31.434	0.243	24	118	63	79	131	137 original
16902	83 Sorbitol	64	[789; Tyramine (3TMS)]	57	0.315	0.162	19.950	0.289	25	117	48	96	73	134 duplicate
14805	83 Sorbitol	41	[639; Proline (2TMS)]	58	0.312	0.162	11.575	0.347	26	116	45	97	20	101 duplicate
17875	83 Sorbitol	57	Mannose	57	0.311	-0.013	25.213	0.338	27	115	76	66	108	107 duplicate
14705	83 Sorbitol	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	58	0.298	-0.037	16.133	0.427	28	114	77	65	45	44 duplicate
17748	83 Sorbitol	76	Fructose	58	0.296	-0.084	14.897	0.330	29	113	86	56	36	114 duplicate
16588	83 Sorbitol	60	Glycerol-3-phosphate	58	0.290	0.595	6.811	0.529	30	112	11	131	1	13 duplicate
14295	83 Sorbitol	36	[596; N-Acetylglutamic acid (2TMS)]	58	0.286	0.693	10.355	0.568	31	111	4	138	11	3 duplicate
17127	83 Sorbitol	67	Citric acid	58	0.278	0.549	8.194	0.440	32	110	14	128	4	42 duplicate
8261	83 Sorbitol	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	57	0.274	-0.088	32.184	0.370	33	109	87	55	132	83 original
17343	83 Sorbitol	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	53	0.271	-0.103	9.385	0.411	34	108	89	53	7	51 duplicate
8235	83 Sorbitol	86	[793; D-Galactono-1,4-lactone (4TMS)]	55	0.271	-0.189	22.860	0.378	35	107	101	41	95	74 original
8286	83 Sorbitol	137	Ergosterol	58	0.269	0.239	13.786	0.370	36	106	40	102	32	82 original
8274	83 Sorbitol	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	58	0.268	-0.128	17.202	0.341	37	105	91	51	50	105 original
14502	83 Sorbitol	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	58	0.267	-0.268	18.114	0.366	38	104	108	34	58	85 duplicate
8271	83 Sorbitol	122	[644; Erythritol (4TMS)]	46	0.264	0.007	28.446	0.391	39	103	73	69	122	61 original
8266	83 Sorbitol	117	[724; Glycerol (3TMS)]	50	0.264	0.085	20.929	0.380	40	102	62	80	79	72 original
17053	83 Sorbitol	66	Glyceric acid-3-phosphate	58	0.263	0.688	20.448	0.530	41	101	7	135	77	12 duplicate
11370	83 Sorbitol	11	Succinic acid	58	0.261	-0.261	17.357	0.367	42	100	107	35	52	84 duplicate
8259	83 Sorbitol	110	[715; Erythritol (4TMS)]	48	0.261	0.080	23.844	0.461	43	99	64	78	101	34 original
16747	83 Sorbitol	62	[812; D-Xylofuranose (4TMS)]	58	0.260	-0.237	12.024	0.331	44	98	105	37	22	111 duplicate

17617	83 Sorbitol	74 [912; Tetradecanoic acid (1TMS)]	58 0,257	0,163	22,397	0,384	45	97	44	98	91	69 duplicate
15099	83 Sorbitol	44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	44 0,254	0,098	17,150	0,344	46	96	58	84	49	102 duplicate
13200	83 Sorbitol	26 Citramalic acid	58 0,251	-0,137	9,659	0,355	47	94	93	49	8	95 duplicate
11754	83 Sorbitol	14 Fumaric acid	58 0,251	-0,220	25,260	0,391	48	95	102	40	110	60 duplicate
8255	83 Sorbitol	106 [733; Threitol (4TMS)]	56 0,248	0,009	19,259	0,454	49	93	72	70	68	36 original
13539	83 Sorbitol	29 Erythritol	58 0,247	-0,354	20,594	0,423	50	92	124	18	78	46 duplicate
8261	83 Sorbitol	132 [895; Isomaltose methoxyamine (8TMS)]	37 0,246	-0,225	27,343	0,212	51	91	103	39	118	140 original
8247	83 Sorbitol	98 [897; Ribose-5-phosphate methoxyamine (5TMS)]	43 0,243	0,283	29,986	0,462	52	90	32	110	128	33 original
12615	83 Sorbitol	21 [878; N,N-DH-(2-Hydroxyethyl)-methanamine (2TMS)]	58 0,235	-0,163	10,711	0,398	53	89	97	45	13	56 duplicate
12734	83 Sorbitol	22 [890; N,N-DH-(2-Hydroxyethyl)-methanamine (2TMS)]	46 0,233	-0,254	26,885	0,327	54	88	106	36	113	115 duplicate
14398	83 Sorbitol	37 Phenylalanine	58 0,230	0,474	7,851	0,477	55	87	19	123	2	27 duplicate
8290	83 Sorbitol	141 Lanosta-8,24-dien-3 $\beta$ -ol	56 0,230	0,141	28,983	0,363	56	86	51	91	126	87 original
16425	83 Sorbitol	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	58 0,223	0,570	8,649	0,550	57	85	13	129	5	5 duplicate
11890	83 Sorbitol	15 Alanine	58 0,214	0,112	10,774	0,385	58	83	55	87	14	68 duplicate
17837	83 Sorbitol	79 Glucose	58 0,214	0,088	17,490	0,468	59	84	61	81	54	29 duplicate
17683	83 Sorbitol	75 Lysine	58 0,208	0,724	20,116	0,538	60	82	3	139	76	7 duplicate
8245	83 Sorbitol	86 myo-Inositol	46 0,202	0,033	34,014	0,373	61	81	88	74	135	78 original
10710	83 Sorbitol	6 Glycerol	58 0,195	-0,059	22,608	0,314	62	80	84	58	92	123 duplicate
12969	83 Sorbitol	24 [725; 2-Ketooctanoic acid (2TMS)]	58 0,183	-0,330	16,230	0,376	64	78	120	22	46	76 duplicate
11499	83 Sorbitol	12 Glycemic acid	57 0,178	-0,294	27,272	0,375	65	77	114	28	117	77 duplicate
8237	83 Sorbitol	88 Gluconic acid	58 0,175	-0,358	18,974	0,401	66	76	128	16	65	54 original
8289	83 Sorbitol	140 [892; Ergosta-7,22-dien-3-ol (1TMS)]	44 0,171	0,055	29,389	0,400	67	75	65	77	127	55 original
12005	83 Sorbitol	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	58 0,169	-0,355	12,555	0,397	68	74	125	17	25	57 duplicate
8285	83 Sorbitol	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	16 0,167	0,493	10,647	0,226	69	73	17	125	12	139 original
12129	83 Sorbitol	17 [700; 2-methyl-1,2-propanediol (2TMS)]	58 0,147	-0,301	13,692	0,378	70	72	117	25	31	73 duplicate
8273	83 Sorbitol	124 [734; 1-Monooleoylglycerol (2TMS); 1-Monoheptadecenoylethanol (1TMS)]	53 0,147	0,177	36,911	0,362	71	71	43	99	140	89 original
10164	83 Sorbitol	2 Serine	58 0,145	0,617	9,668	0,569	72	70	9	133	9	2 duplicate
14804	83 Sorbitol	39 [829; 1-Phenylethanol (1TMS)]	57 0,145	-0,293	19,192	0,358	73	69	113	29	67	92 duplicate
16978	83 Sorbitol	65 [646; 3-Deoxyglucitol (5TMS)]	57 0,140	-0,277	27,638	0,349	74	68	109	33	120	100 duplicate
8276	83 Sorbitol	127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	33 0,136	-0,143	15,801	0,132	75	67	94	48	42	141 original
18258	83 Sorbitol	56 [828; Orolic acid (3TMS)]	58 0,138	-0,284	26,481	0,362	76	68	115	27	112	91 duplicate
15290	83 Sorbitol	46 Arabinose	58 0,132	-0,289	21,571	0,356	77	65	112	30	82	94 duplicate
8269	83 Sorbitol	120 [945; Uridine (3TMS)]	48 0,126	-0,280	12,824	0,357	78	64	110	32	27	93 original
17200	83 Sorbitol	68 [570; Hypoxanthine (2TMS)]	18 0,124	0,126	21,432	0,393	79	63	53	89	81	59 duplicate
8283	83 Sorbitol	134 Isomaltose	58 0,116	-0,302	17,934	0,362	80	62	118	24	55	90 original
16014	83 Sorbitol	54 [NA]	49 0,114	-0,353	27,042	0,317	81	61	123	19	116	122 duplicate
11109	83 Sorbitol	9 Proline	57 0,112	0,645	11,002	0,555	82	60	8	134	17	4 duplicate
13760	83 Sorbitol	31 [622; Parabanic acid (2TMS)]	58 0,101	0,388	24,651	0,444	83	59	25	117	106	41 duplicate
8241	83 Sorbitol	92 [680; Glycero-2-phosphate (4TMS)]	48 0,089	-0,168	20,937	0,261	84	58	99	43	80	136 original
8267	83 Sorbitol	118 [928; Glucopyranose-6-phosphate (6TMS)]	52 0,072	0,093	21,747	0,298	85	57	60	82	85	130 original
8279	83 Sorbitol	130 Trehalose	57 0,069	0,240	12,579	0,380	86	56	38	104	26	71 original
8288	83 Sorbitol	139 [700; Ergosta-5,7-dien-3-ol]	33 0,088	0,038	28,813	0,337	87	55	67	75	124	108 original
15660	83 Sorbitol	50 [746; Ribonic acid-1,4-lactone (3TMS)]	55 0,067	-0,388	34,713	0,377	88	54	129	13	136	75 duplicate
12852	83 Sorbitol	23 Homoserine	58 0,061	-0,233	17,984	0,445	89	53	41	101	57	40 duplicate
8277	83 Sorbitol	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	39 0,061	-0,229	16,122	0,232	90	52	104	38	44	138 original
10302	83 Sorbitol	3 Ethanolamine	56 0,057	0,403	24,044	0,470	91	51	23	119	103	28 duplicate
11627	83 Sorbitol	13 Uracil	58 0,053	-0,361	15,373	0,397	92	50	127	15	39	58 duplicate
8252	83 Sorbitol	103 [648; Ethylamine (2TMS)]	57 0,051	-0,385	22,665	0,465	93	49	128	14	94	30 original

16342	83 Sorbitol	57	[757]: 2-Desoxy-pentos-3-ylose dimethoxyamine (2TMS)]	49	0,046	-0,304	21,708	0,303	94	48	119	23	84	127 duplicate
		129	[840]: Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]											
8276	83 Sorbitol	81	Tyrosine	53	0,044	-0,349	24,171	0,321	95	47	122	20	104	120 original
18058	83 Sorbitol	58	[815]: (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	58	0,032	0,501	16,041	0,531	96	46	16	126	43	10 duplicate
13314	83 Sorbitol	49	Methionine	49	0,028	0,272	28,603	0,480	97	45	34	108	123	26 duplicate
13977	83 Sorbitol	58	[826]: beta-[[[5-methyl-2-thenyl)methylethylamino- benzeneacetic acid methyl ester]	58	0,025	0,319	17,432	0,412	98	44	28	113	53	60 duplicate
		77	[826]: beta-[[[5-methyl-2-thenyl)methylethylamino- benzeneacetic acid methyl ester]	57	0,008	0,477	12,659	0,502	99	43	18	124	28	17 duplicate
17812	83 Sorbitol	30	[815]: Ethyl-3(2H)-thiophenone]	58	0,007	0,409	13,180	0,446	100	42	22	120	30	39 duplicate
13650	83 Sorbitol	32	[729]: N,N-Dimethyllysine methyl ester]	57	0,005	0,440	24,955	0,498	101	41	20	122	107	19 duplicate
13869	83 Sorbitol	80	[772]: D-Glucose (5TMS)]	56	0,001	-0,095	16,918	0,292	102	40	88	54	48	133 duplicate
17898	83 Sorbitol	34	Aspartic acid	58	0,001	0,294	15,056	0,372	103	39	31	111	37	79 duplicate
14084	83 Sorbitol	4	Phosphoric acid	51	-0,001	0,734	13,887	0,504	104	38	1	141	34	15 duplicate
10439	83 Sorbitol	87	[945]: beta-D-Glucopyranose (5TMS)]	57	-0,004	-0,180	20,047	0,322	105	37	100	42	75	118 original
8236	83 Sorbitol	59	Ornithine; Arginine	58	-0,007	0,536	21,576	0,483	106	36	15	127	83	25 duplicate
16507	83 Sorbitol	119	[931]: myo-Inositol-2-phosphate (7TMS)]	58	-0,039	-0,055	18,474	0,293	107	35	82	60	61	131 original
8268	83 Sorbitol	107	9-(Z)-Octadecenoic acid	52	-0,048	-0,070	11,142	0,331	108	34	85	57	18	110 original
8256	83 Sorbitol	8	Isoleucine	52	-0,051	0,682	8,193	0,587	109	33	5	137	3	1 duplicate
10977	83 Sorbitol	108	Octadecenoic acid	58	-0,053	0,122	21,979	0,350	110	32	54	88	89	99 original
8257	83 Sorbitol	101	[832]: Dopamine (4TMS)]	58	-0,060	-0,392	21,887	0,497	111	31	130	12	86	21 original
8250	83 Sorbitol	105	[705]: 2-Ketogluconic acid (5TMS)]	42	-0,082	-0,434	19,333	0,388	112	30	133	9	69	65 original
8254	83 Sorbitol	10	Glycine	58	-0,083	0,283	9,705	0,386	113	29	33	109	10	67 duplicate
11240	83 Sorbitol	45	Homocysteine	55	-0,099	0,040	35,649	0,353	114	28	66	76	138	98 duplicate
15195	83 Sorbitol	51	[499]: 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	43	-0,105	0,332	32,822	0,462	115	27	28	114	134	32 duplicate
15750	83 Sorbitol	61	[NA]	48	-0,112	0,032	18,951	0,288	116	26	69	73	64	135 duplicate
16668	83 Sorbitol	52	[NA]	40	-0,121	0,010	28,896	0,434	117	25	75	67	125	43 duplicate
15839	83 Sorbitol	95	[770]: 3,4,6-Tris-hydroxyphenylethanolamine (5TMS)]	44	-0,121	0,101	30,319	0,331	118	24	57	85	129	112 original
8244	83 Sorbitol	69	Arginine	55	-0,126	0,271	10,776	0,462	119	23	35	107	15	31 duplicate
15477	83 Sorbitol	48	Asparagine	58	-0,139	0,138	19,483	0,365	120	22	52	90	71	86 duplicate
8240	83 Sorbitol	91	[766]: beta-D-Methylglucopyranoside (4TMS)]	58	-0,145	-0,562	26,351	0,530	121	21	136	6	111	11 original
14904	83 Sorbitol	42	Glutamic acid	55	-0,149	-0,412	14,432	0,498	122	20	21	121	35	20 duplicate
15002	83 Sorbitol	43	[548]: Leucine (2TBS)]	54	-0,159	-0,049	17,327	0,335	123	19	80	62	51	109 duplicate
8246	83 Sorbitol	97	[756]: beta-D-Methylglucopyranoside (4TMS)]	46	-0,171	-0,493	19,973	0,455	124	18	135	7	74	35 original
8239	83 Sorbitol	90	[910]: 9-(Z)-Hexadecenoic acid (1TMS)]	58	-0,218	-0,299	18,467	0,344	125	17	116	26	60	103 original
17482	83 Sorbitol	72	[919]: D-Xylopyranose (4TMS)]	57	-0,226	-0,133	23,246	0,363	126	16	92	50	98	88 duplicate
13085	83 Sorbitol	25	[709]: 2,5-Diaminovalerolactam (2TMS)]	42	-0,226	-0,133	23,246	0,363	126	16	92	50	98	88 duplicate
8248	83 Sorbitol	99	[662]: Ribose-5-phosphate methoxyamine (BP) (5TMS)]	35	-0,230	-0,410	22,938	0,414	127	15	42	100	93	49 duplicate
16825	83 Sorbitol	63	Glutamine	46	-0,241	0,010	24,502	0,288	128	14	132	10	96	132 original
8238	83 Sorbitol	89	[775]: Dopamine (4TMS)]	34	-0,276	-0,056	25,250	0,447	130	12	83	59	109	38 original
16100	83 Sorbitol	55	[612]: 4-Aminobutyric acid (2TBS)]	43	-0,278	-0,284	36,630	0,495	131	11	111	31	139	22 duplicate
8260	83 Sorbitol	131	[626]: 5-Methylthiadenosine (3TMS)]	51	-0,285	-0,161	30,809	0,354	132	10	98	46	130	97 original
15569	83 Sorbitol	49	[877]: Pyrophosphoric acid (4TMS)]	58	-0,319	-0,105	34,761	0,343	133	9	90	52	137	104 duplicate
15927	83 Sorbitol	53	Glycerol-2-phosphate	58	-0,337	-0,334	26,915	0,301	134	8	121	21	114	128 duplicate
8242	83 Sorbitol	93	[607]: Putrescine (4TMS)]	54	-0,371	-0,366	32,175	0,501	135	7	131	11	133	18 original
8233	83 Sorbitol	84	Mannitol	56	-0,397	-0,770	18,782	0,534	136	6	139	3	62	9 original
15394	83 Sorbitol	47	[NA]	58	-0,429	-0,490	23,325	0,408	137	5	134	8	99	52 duplicate
10025	83 Sorbitol	1	[938]: Sulfuric acid (2TMS)]	30	-0,471	-0,695	19,340	0,380	138	4	137	5	70	64 duplicate
10575	83 Sorbitol	5	Leucine	45	-0,493	-0,718	23,492	0,535	139	3	138	4	100	8 duplicate
18117	83 Sorbitol	82	Lysine	39	-0,536	-0,839	15,068	0,519	140	2	141	1	38	14 duplicate

12495	83 Sorbitol	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.604	-0.782	26.917	0.489	141	1	140	2	115	23 duplicate
10026	84 Mannitol	34	[938; Sulfuric acid (2TMS)]	34	0.533	0.769	25.585	0.584	1	141	2	140	62	5 duplicate
8289	84 Mannitol	58	[607; Putrescine (4TMS)]	58	0.528	0.680	40.067	0.470	2	140	5	137	128	58 original
18118	84 Mannitol	82	Lysine	37	0.468	0.617	11.686	0.531	3	139	9	133	2	18 duplicate
8305	84 Mannitol	99	[662; Ribose-5-phosphate methoxamine (BP) (5TMS)]	39	0.449	0.633	31.675	0.548	4	138	8	134	95	10 original
8311	84 Mannitol	105	[705; 2-Ketoglucuronic acid (5TMS)]	46	0.447	0.773	21.577	0.518	5	137	1	141	43	23 original
16101	84 Mannitol	55	[612; 4-Aminobutyric acid (2TBS)]	42	0.415	0.465	36.730	0.485	6	136	30	112	115	51 duplicate
12496	84 Mannitol	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	0.389	0.608	27.478	0.487	7	135	10	132	74	49 duplicate
16015	84 Mannitol	54	[NA]	53	0.380	0.584	34.164	0.472	8	134	12	130	105	57 duplicate
10576	84 Mannitol	5	Leucine	43	0.367	0.389	21.648	0.507	8	133	36	106	44	30 duplicate
8298	84 Mannitol	80	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	62	0.355	0.352	27.676	0.355	10	132	42	100	76	131 original
8334	84 Mannitol	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	43	0.344	0.551	23.315	0.441	11	131	16	126	51	83 original
8298	84 Mannitol	82	[680; Glycerol-2-phosphate (4TMS)]	52	0.335	0.372	28.732	0.404	12	130	38	104	80	106 original
16343	84 Mannitol	57	[757; 2-Desoxy-pentose-3-yose dimethoxamine (2TMS)]	53	0.325	0.468	25.707	0.460	13	129	28	114	63	73 duplicate
8303	84 Mannitol	97	[756; beta-D-Methylglucopyranoside (4TMS)]	50	0.304	0.708	16.145	0.607	14	128	4	138	14	2 original
8341	84 Mannitol	135	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	62	0.301	0.321	21.924	0.414	15	127	45	97	45	100 original
11500	84 Mannitol	61	Glyceric acid	61	0.296	0.547	37.190	0.420	16	126	18	124	116	94 duplicate
8318	84 Mannitol	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	61	0.277	0.366	43.413	0.423	17	125	39	103	135	93 original
13540	84 Mannitol	29	Erythritol	62	0.263	0.588	30.319	0.498	18	124	11	131	86	37 duplicate
8313	84 Mannitol	107	9-(Z)-Octadecenoic acid	62	0.252	0.062	20.342	0.348	19	123	66	76	38	133 original
16385	84 Mannitol	47	[NA]	62	0.231	0.551	28.711	0.498	20	122	17	125	79	38 duplicate
16826	84 Mannitol	63	Glutamine	50	0.231	-0.020	35.821	0.437	21	121	77	65	113	85 duplicate
15291	84 Mannitol	46	Arabinose	62	0.225	0.455	24.538	0.458	22	120	31	111	56	74 duplicate
12006	84 Mannitol	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	62	0.222	0.568	16.683	0.494	23	119	14	128	19	43 duplicate
15661	84 Mannitol	50	[746; Ribonic acid-1,4-lactone (3TMS)]	59	0.222	0.575	44.269	0.509	24	118	13	129	138	28 duplicate
11371	84 Mannitol	11	Succinic acid	62	0.219	0.471	26.621	0.432	25	117	27	115	68	87 duplicate
14605	84 Mannitol	39	[829; 1-Phenylethanol (1TMS)]	61	0.217	0.505	22.581	0.448	26	116	23	119	48	79 duplicate
12970	84 Mannitol	24	[725; 2-Ketooctanoic acid (2TMS)]	62	0.213	0.529	10.267	0.478	27	115	19	123	1	54 duplicate
11628	84 Mannitol	13	Uracil	62	0.211	0.555	19.142	0.495	28	114	15	127	30	41 duplicate
8335	84 Mannitol	129	[840; Maltose methoxamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	57	0.209	0.499	28.759	0.468	29	113	25	117	84	62 original
16979	84 Mannitol	65	[646; 3-Deoxyglucitol (5TMS)]	61	0.209	0.450	33.775	0.453	30	112	32	110	103	77 duplicate
12616	84 Mannitol	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	62	0.194	0.354	18.162	0.426	31	110	41	101	26	92 duplicate
8325	84 Mannitol	119	[931; myo-Inositol-2-phosphate (7TMS)]	62	0.194	0.144	28.538	0.335	32	111	57	85	77	138 original
12735	84 Mannitol	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	50	0.190	0.527	35.538	0.434	33	109	20	122	111	86 duplicate
16748	84 Mannitol	62	[612; D-Xylofuranose (4TMS)]	62	0.186	0.401	20.110	0.428	34	108	35	107	38	90 duplicate
8295	84 Mannitol	89	[775; Dopamine (4TMS)]	34	0.184	0.086	29.529	0.461	35	107	64	78	83	69 original
14503	84 Mannitol	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	62	0.182	0.500	26.963	0.461	36	106	24	118	70	68 duplicate
8340	84 Mannitol	134	Isomaltose	62	0.180	0.482	16.235	0.468	37	105	26	116	16	60 original
8287	84 Mannitol	91	[766; beta-D-Methylglucopyranoside (4TMS)]	62	0.179	0.768	26.267	0.548	38	104	3	139	67	9 original
16259	84 Mannitol	56	[829; Optic acid (3TMS)]	62	0.177	0.468	33.597	0.464	39	103	29	113	101	66 duplicate
8306	84 Mannitol	100	[857; Mannitol (6TMS)]	62	0.176	0.354	25.595	0.419	40	102	40	102	61	96 original
15928	84 Mannitol	53	Glycerol-2-phosphate	82	0.174	0.299	37.379	0.389	41	101	47	95	118	114 duplicate
8308	84 Mannitol	102	[904; Galactose methoxamine (5TMS)]	62	0.172	0.280	32.594	0.395	42	100	48	94	97	110 original
8338	84 Mannitol	132	[895; Isomaltose methoxamine (8TMS)]	40	0.172	0.416	35.653	0.417	43	99	34	108	112	98 original
8326	84 Mannitol	120	[945; Uridine (3TMS)]	52	0.166	0.219	21.471	0.462	44	98	50	92	42	67 original
12130	84 Mannitol	17	[700; 2-methyl-1,2-propanediol (2TMS)]	62	0.166	0.511	17.600	0.484	45	96	22	120	24	53 duplicate

16669	84 Mannitol	61 [NA]	62 0.166	0.062	29.807	0.393	46	97	67	75	85	111 duplicate
8307	84 Mannitol	101 [832; Dopamine (4TMS)]	62 0.159	0.678	26.941	0.484	47	95	6	136	69	52 original
8294	84 Mannitol	88 Gluconic acid	62 0.157	0.524	24.510	0.525	48	94	21	121	55	18 original
15570	84 Mannitol	49 [877; Pyrophosphoric acid (4TMS)]	62 0.153	0.142	44.234	0.378	49	93	59	83	137	123 duplicate
8309	84 Mannitol	103 [648; Ethylamine (2TMS)]	61 0.150	0.650	25.842	0.519	50	92	7	135	65	20 original
11755	84 Mannitol	14 Fumaric acid	62 0.150	0.435	35.483	0.445	51	91	33	109	110	80 duplicate
8333	84 Mannitol	127 [777; Fructose-6-phosphate methoxymamine (6TMS)]	37 0.132	0.345	25.981	0.411	52	90	43	99	68	102 original
8292	84 Mannitol	86 [793; D-Galactono-1,4-lactone (4TMS)]	59 0.127	0.321	24.431	0.466	53	89	44	98	54	64 original
13428	84 Mannitol	28 Malic acid	62 0.119	0.387	24.923	0.444	54	88	37	105	58	81 duplicate
15840	84 Mannitol	52 [NA]	44 0.110	0.006	42.153	0.625	55	87	74	68	133	1 duplicate
13201	84 Mannitol	26 Citramalic acid	62 0.105	0.318	18.267	0.400	56	86	46	96	27	109 duplicate
17618	84 Mannitol	74 [912; Tetradecanoic acid (1TMS)]	62 0.099	-0.067	33.888	0.415	57	85	86	56	104	99 duplicate
14708	84 Mannitol	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	62 0.087	0.199	12.397	0.495	59	83	51	91	3	39 duplicate
8291	84 Mannitol	85 [529; Methylenic acid (4TMS)]	46 0.078	-0.045	19.100	0.503	60	82	81	61	29	32 original
8337	84 Mannitol	131 [626; 5-Methylthiadenosine (3TMS)]	53 0.061	-0.004	40.283	0.429	61	81	76	66	129	89 original
8314	84 Mannitol	108 Octadecanoic acid	62 0.059	-0.237	33.525	0.359	62	80	98	44	100	129 original
15751	84 Mannitol	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44 0.057	-0.403	39.210	0.491	63	79	106	36	124	47 duplicate
8301	84 Mannitol	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50 0.055	-0.110	44.187	0.331	64	78	90	52	136	139 original
17483	84 Mannitol	72 [919; D-Xylopyranose (4TMS)]	61 0.054	0.109	32.864	0.347	65	77	63	79	98	135 duplicate
12253	84 Mannitol	18 [590; 1-Acetyl-2-thiohydantoin]	62 0.051	0.000	27.547	0.375	66	76	75	67	75	124 duplicate
8331	84 Mannitol	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	62 0.043	0.148	15.104	0.401	67	75	55	87	10	108 original
8347	84 Mannitol	141 Lanosta-8,24-dien-3-beta-ol	59 0.036	-0.037	38.830	0.364	68	74	80	62	123	127 original
15100	84 Mannitol	44 [910; 2-Ketogluconic acid methoxymamine (4TMS)]	48 0.027	0.027	27.316	0.493	69	73	71	73	44 duplicate	
8293	84 Mannitol	87 [945; beta-D-Glucopyranose (5TMS)]	60 0.019	0.180	15.946	0.413	70	72	52	90	13	101 original
8321	84 Mannitol	115 Glucose-6-phosphate	60 0.011	0.118	14.437	0.418	71	71	61	81	5	97 original
8328	84 Mannitol	122 [644; Erythritol (4TMS)]	50 0.011	0.167	38.680	0.542	72	70	53	89	122	12 original
17749	84 Mannitol	76 Fructose	62 0.006	0.143	16.860	0.402	73	69	58	84	21	107 duplicate
8317	84 Mannitol	111 [583; Erythritol (4TMS)]	40 0.003	-0.086	41.285	0.358	74	68	87	55	132	130 original
15478	84 Mannitol	48 Asparagine	62 0.002	-0.235	31.284	0.464	75	67	97	45	94	65 duplicate
8346	84 Mannitol	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	47 -0.001	0.036	37.508	0.344	76	66	70	72	119	136 original
8316	84 Mannitol	110 [715; Erythritol (4TMS)]	52 -0.008	0.058	34.171	0.600	77	65	68	74	106	4 original
15186	84 Mannitol	45 Homocysteine	60 -0.008	-0.057	48.043	0.410	78	64	83	59	139	103 duplicate
8332	84 Mannitol	128 [559; Erythritol (4TMS)]	-43 -0.012	-0.164	30.778	0.569	79	63	93	49	87	6 original
8343	84 Mannitol	137 Ergosterol	62 -0.015	-0.310	25.759	0.342	80	62	100	42	64	137 original
17876	84 Mannitol	78 Mannose	60 -0.018	0.124	34.654	0.369	81	61	60	82	109	128 duplicate
8322	84 Mannitol	116 [882; Pseudouridine (5TMS)]	28 -0.021	0.158	19.496	0.441	82	60	54	88	32	84 original
8312	84 Mannitol	106 [733; Threitol (4TMS)]	60 -0.032	0.083	28.890	0.554	83	59	65	77	81	8 original
8345	84 Mannitol	69 Arginine	58 -0.032	-0.483	21.010	0.504	84	58	114	28	40	31 duplicate
15003	84 Mannitol	139 [700; Ergosta-5,7-dien-3-ol]	36 -0.035	-0.058	38.260	0.348	85	57	85	57	121	134 original
8323	84 Mannitol	43 [548; Leucine (2TBS)]	59 -0.039	-0.028	27.080	0.387	86	56	79	63	71	115 duplicate
14191	84 Mannitol	117 [724; Glycerol (3TMS)]	54 -0.040	0.026	31.882	0.494	87	55	72	70	96	42 original
17128	84 Mannitol	35 Pyroglutamic acid	62 -0.043	0.145	16.313	0.405	88	54	56	86	18	105 duplicate
8327	84 Mannitol	67 Citric acid	62 -0.045	-0.567	14.663	0.489	89	53	121	21	7	48 duplicate
17344	84 Mannitol	121 [657; Erythritol (4TMS)]	53 -0.046	-0.057	39.300	0.427	90	52	84	58	125	91 original
13086	84 Mannitol	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	55 -0.052	-0.023	16.291	0.389	91	51	78	64	17	113 duplicate
8302	84 Mannitol	25 [709; 2,5-Diaminovalerolactam (2TMS)]	46 -0.057	-0.480	36.892	0.496	92	50	113	29	114	36 duplicate
8315	84 Mannitol	96 myo-Inositol	47 -0.066	0.052	40.392	0.318	93	49	69	73	130	140 original
16589	84 Mannitol	109 Octadecanoic acid	62 -0.068	-0.381	23.450	0.375	94	48	103	39	52	125 original
14400	84 Mannitol	60 Glycerol-3-phosphate	62 -0.094	-0.603	17.359	0.559	95	47	123	19	23	7 duplicate
		37 Phenylalanine	62 -0.096	-0.612	15.776	0.515	96	46	125	17	11	25 duplicate

17613	84 Mannitol	[826; beta-[[[5-methyl-2-thienyl]methyl]eneamino- benzeneacetic acid methyl ester]	60	-0.088	-0.634	22.347	0.495	97	45	127	15	46	40 duplicate
8300	84 Mannitol	Hexadecanoic acid	62	-0.103	-0.358	19.623	0.392	98	44	101	41	34	112 original
17999	84 Mannitol	[772; D-Glucose (5TMS)]	61	-0.109	0.111	15.940	0.386	99	43	62	80	12	116 duplicate
11241	84 Mannitol	Glycine	62	-0.119	-0.446	21.169	0.474	100	42	112	30	41	55 duplicate
10711	84 Mannitol	Glycerol	62	-0.120	0.022	16.961	0.429	101	41	73	69	22	88 duplicate
10978	84 Mannitol	8 Isoleucine	53	-0.123	-0.753	22.786	0.461	102	40	133	9	49	70 duplicate
14905	84 Mannitol	Glutamic acid	58	-0.129	-0.711	24.705	0.501	103	39	131	11	57	33 duplicate
10303	84 Mannitol	Ethanolamine	60	-0.130	-0.495	37.352	0.520	104	38	116	26	117	19 duplicate
18059	84 Mannitol	Tyrosine	62	-0.139	-0.626	20.642	0.607	105	37	126	16	39	3 duplicate
8330	84 Mannitol	[734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	57	-0.152	-0.423	49.729	0.382	106	36	109	33	140	118 original
14806	84 Mannitol	[639; Proline (2TMS)]	62	-0.155	-0.221	22.534	0.420	107	35	96	46	47	95 duplicate
12375	84 Mannitol	Alanine (BP) (3TMS)	62	-0.156	-0.159	24.927	0.444	108	34	92	50	59	82 duplicate
14085	84 Mannitol	Aspartic acid	62	-0.157	-0.405	16.696	0.378	109	32	107	35	20	122 duplicate
13978	84 Mannitol	Methionine	62	-0.157	-0.429	31.177	0.408	110	33	110	32	92	104 duplicate
8319	84 Mannitol	113 Galactose-6-phosphate	60	-0.163	-0.048	34.285	0.508	111	31	82	60	108	29 original
16508	84 Mannitol	Ornithine; Arginine	62	-0.173	-0.655	19.522	0.492	112	30	128	14	33	45 duplicate
13651	84 Mannitol	[815; Ethyl-3(2H)-thiophenone]	62	-0.175	-0.536	20.034	0.450	113	29	118	24	35	78 duplicate
8342	84 Mannitol	[748; D-Sedoheptulose-7-phosphate (7TMS)]	16	-0.183	-0.377	15.058	0.303	114	28	102	40	9	141 original
17414	84 Mannitol	[731; Erythrose (3TMS)]	62	-0.184	-0.608	23.108	0.515	115	27	124	18	50	26 duplicate
8339	84 Mannitol	[855; Squalene]	62	-0.185	-0.432	30.813	0.383	116	26	111	31	88	117 original
17551	84 Mannitol	[708; Glucose methoxamine (5TMS)]	55	-0.189	-0.092	31.005	0.381	117	25	88	54	90	120 duplicate
8324	84 Mannitol	[928; Glucopyranose-6-phosphate (6TMS)]	56	-0.196	-0.151	33.320	0.379	118	24	91	51	99	121 original
16903	84 Mannitol	[789; Tyramine (3TMS)]	61	-0.201	-0.175	31.249	0.359	119	23	94	48	93	128 duplicate
8320	84 Mannitol	Fructose-6-phosphate	51	-0.208	-0.104	34.175	0.546	120	22	89	53	107	11 original
12853	84 Mannitol	23 Homoserine	62	-0.229	-0.491	30.979	0.473	121	21	115	27	89	58 duplicate
13870	84 Mannitol	[729; N,N-Dimethyllysine methyl ester]	61	-0.259	-0.691	40.670	0.515	122	20	130	12	131	24 duplicate
11881	84 Mannitol	Alanine	62	-0.265	-0.253	20.162	0.468	123	19	99	43	37	61 duplicate
13761	84 Mannitol	[622; Parabanic acid (2TMS)]	61	-0.267	-0.662	37.846	0.491	124	18	129	13	120	48 duplicate
8310	84 Mannitol	[795; Erythritol (4TMS)]	61	-0.268	-0.389	31.055	0.467	125	17	105	37	91	63 original
13315	84 Mannitol	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	52	-0.279	-0.564	39.703	0.457	126	16	120	22	126	76 duplicate
8344	84 Mannitol	[874; Ergosterol (1TMS)]	44	-0.281	-0.527	39.755	0.382	127	15	117	25	127	119 original
17201	84 Mannitol	[570; Hypoxanthine (2TMS)]	19	-0.287	-0.387	29.370	0.457	128	14	104	38	82	75 duplicate
10440	84 Mannitol	4 Phosphoric acid	49	-0.294	-0.761	14.826	0.460	129	13	134	8	8	72 duplicate
10845	84 Mannitol	Threonine	62	-0.306	-0.717	14.460	0.469	130	12	132	10	6	59 duplicate
17938	84 Mannitol	Glucose	62	-0.320	-0.201	16.224	0.514	131	11	95	47	15	27 duplicate
14296	84 Mannitol	[596; N-Acetylglutamic acid (2TMS)]	62	-0.321	-0.838	18.028	0.542	132	10	140	2	25	13 duplicate
8304	84 Mannitol	[697; Ribose-5-phosphate methoxamine (5TMS)]	47	-0.321	-0.539	42.916	0.461	133	9	119	23	134	71 original
11110	84 Mannitol	Proline	61	-0.322	-0.822	27.145	0.499	134	8	139	3	72	35 duplicate
17054	84 Mannitol	Glyceric acid-3-phosphate	62	-0.323	-0.779	33.666	0.542	135	7	136	6	102	14 duplicate
8329	84 Mannitol	[945; Galactofuranose-6-phosphate (7TMS)]	62	-0.350	-0.417	25.069	0.517	136	6	108	34	60	21 original
8336	84 Mannitol	130 Trehalose	61	-0.393	-0.575	13.735	0.500	137	5	122	20	4	34 original
18176	84 Mannitol	Sorbitol	56	-0.397	-0.770	18.782	0.534	138	4	135	7	28	15 duplicate
10165	84 Mannitol	2 Serine	60	-0.409	-0.808	26.566	0.486	139	3	138	4	78	50 duplicate
17684	84 Mannitol	Lysine	62	-0.539	-0.863	19.302	0.517	140	2	141	1	31	22 duplicate
16426	84 Mannitol	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	62	-0.608	-0.793	24.286	0.530	141	1	137	5	53	17 duplicate
8394	85 [529; Methylcitric acid (4 132	[895; Isomaltose methoxamine (8TMS)]	27	0.664	0.849	14.163	0.374	1	141	2	140	91	128 original
17619	85 [529; Methylcitric acid (4 74	[912; Tetradecanoic acid (1TMS)]	48	0.637	0.854	7.785	0.579	2	140	1	141	36	10 duplicate
8371	85 [529; Methylcitric acid (4 109	Octadecanoic acid	48	0.624	0.849	19.913	0.486	3	139	3	139	118	66 original

8400	85 [529; Methyldiictric acid (4 138 [674; Ergosterol (1TMS)]	34	0.601	0.755	10,727	0.534	4	138	13	129	68	28 original
8390	85 [529; Methyldiictric acid (4 128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	29	0.571	0.701	4,994	0.388	5	137	30	112	16	121 original
8395	85 [529; Methyldiictric acid (4 133 [855; Squalene]	48	0.571	0.725	4,014	0.571	6	136	22	120	8	14 original
8356	85 [529; Methyldiictric acid (4 94 Hexadecanoic acid	48	0.562	0.834	18,513	0.531	7	135	4	138	111	31 original
13429	85 [529; Methyldiictric acid (4 28 Malic acid	48	0.543	0.818	4,638	0.565	8	134	5	137	15	19 duplicate
16344	85 [529; Methyldiictric acid (4 57 [757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	39	0.541	0.668	9,897	0.420	9	133	39	103	60	108 duplicate
8376	85 [529; Methyldiictric acid (4 114 Fructose-6-phosphate	37	0.535	0.672	6,641	0.441	10	132	37	105	26	97 original
8378	85 [529; Methyldiictric acid (4 116 [882; Pseudouridine (5TMS)]	30	0.531	0.565	7,710	0.324	11	131	60	82	35	138 original
8354	85 [529; Methyldiictric acid (4 92 [680; Glyceral-2-phosphate (4TMS)]	38	0.531	0.471	7,428	0.347	12	130	69	73	31	133 original
8377	85 [529; Methyldiictric acid (4 115 Glucose-6-phosphate	46	0.519	0.642	19,026	0.402	13	129	44	98	113	116 original
8362	85 [529; Methyldiictric acid (4 100 [857; Mannitol (6TMS)]	48	0.516	0.747	4,454	0.460	14	128	16	126	14	84 original
14707	85 [529; Methyldiictric acid (4 40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	48	0.502	0.770	28,296	0.594	15	127	11	131	131	5 duplicate
11756	85 [529; Methyldiictric acid (4 14 Fumaric acid	48	0.498	0.783	6,231	0.498	16	125	10	132	23	55 duplicate
18177	85 [529; Methyldiictric acid (4 83 Sorbitol	48	0.498	0.731	18,803	0.541	17	126	20	122	112	25 duplicate
8375	85 [529; Methyldiictric acid (4 113 Galactose-6-phosphate	46	0.496	0.529	7,171	0.517	18	124	64	78	30	39 original
8389	85 [529; Methyldiictric acid (4 127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	23	0.494	0.622	4,215	0.401	19	123	48	94	10	117 original
8364	85 [529; Methyldiictric acid (4 102 [904; Galactose methoxyamine (5TMS)]	48	0.489	0.699	3,316	0.494	20	122	31	111	7	59 original
12736	85 [529; Methyldiictric acid (4 22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	38	0.482	0.793	10,154	0.481	21	121	7	135	61	69 duplicate
8402	85 [529; Methyldiictric acid (4 140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	40	0.477	0.620	12,233	0.492	22	120	49	93	79	60 original
8403	85 [529; Methyldiictric acid (4 141 Lanosta-8,24-dien-3-beta-ol	48	0.470	0.643	9,680	0.512	23	119	43	99	58	43 original
16016	85 [529; Methyldiictric acid (4 54 [NA]	39	0.468	0.614	10,876	0.397	24	118	52	90	70	119 duplicate
8397	85 [529; Methyldiictric acid (4 902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	48	0.461	0.754	8,200	0.548	25	117	14	128	39	22 original
8388	85 [529; Methyldiictric acid (4 126 [559; Erythritol (4TMS)]	29	0.458	0.815	5,951	0.589	26	116	6	136	22	7 original
16749	85 [529; Methyldiictric acid (4 62 [812; D-Xylofuranose (4TMS)]	48	0.452	0.614	9,203	0.502	27	115	53	89	51	53 duplicate
8367	85 [529; Methyldiictric acid (4 105 [705; 2-Ketogluconic acid (5TMS)]	32	0.452	0.630	5,935	0.509	28	114	46	96	21	48 original
8379	85 [529; Methyldiictric acid (4 117 [724; Glyceral (3TMS)]	40	0.451	0.791	7,055	0.546	29	113	8	134	28	23 original
17415	85 [529; Methyldiictric acid (4 71 [731; Erythrose (3TMS)]	48	0.449	0.656	9,028	0.594	30	112	42	100	47	4 duplicate
8382	85 [529; Methyldiictric acid (4 120 [845; Uridine (3TMS)]	38	0.448	0.354	7,479	0.509	31	111	72	70	33	45 original
8361	85 [529; Methyldiictric acid (4 99 [682; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	25	0.440	0.788	9,583	0.400	33	109	9	133	55	118 original
11372	85 [529; Methyldiictric acid (4 11 Succinic acid	48	0.436	0.664	3,158	0.447	34	108	40	102	6	93 duplicate
8374	85 [529; Methyldiictric acid (4 112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	47	0.434	0.727	12,675	0.507	35	106	21	121	81	48 original
11501	85 [529; Methyldiictric acid (4 70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	47	0.434	0.708	8,445	0.481	36	107	27	115	41	71 duplicate
17345	85 [529; Methyldiictric acid (4 70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	46	0.432	0.535	14,145	0.357	37	105	63	79	90	130 duplicate
8399	85 [529; Methyldiictric acid (4 137 Ergosterol	48	0.429	0.615	10,675	0.487	38	104	51	91	66	65 original
8372	85 [529; Methyldiictric acid (4 110 [715; Erythritol (4TMS)]	38	0.428	0.741	10,688	0.583	39	103	17	125	67	8 original
15662	85 [529; Methyldiictric acid (4 50 [746; Ribonic acid-1,4-lactone (3TMS)]	45	0.424	0.703	15,912	0.447	40	102	29	113	100	94 duplicate
14182	85 [529; Methyldiictric acid (4 35 Pyroglutamic acid	48	0.424	0.566	33,765	0.432	41	101	59	83	138	102 duplicate
8396	85 [529; Methyldiictric acid (4 134 Isomaltose	48	0.418	0.683	15,993	0.473	42	100	34	108	101	76 original
8383	85 [529; Methyldiictric acid (4 121 [657; Erythritol (4TMS)]	39	0.417	0.711	10,750	0.497	43	99	26	116	69	56 original
8394	85 [529; Methyldiictric acid (4 122 [644; Erythritol (4TMS)]	36	0.413	0.759	13,314	0.528	44	98	12	130	84	33 original
14504	85 [529; Methyldiictric acid (4 38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	48	0.410	0.748	3,093	0.466	45	97	15	127	5	80 duplicate
16260	85 [529; Methyldiictric acid (4 56 [829; Orolic acid (3TMS)]	48	0.408	0.639	9,761	0.432	46	96	45	97	59	101 duplicate
11629	85 [529; Methyldiictric acid (4 13 Uracil	48	0.406	0.711	9,174	0.515	47	95	25	117	50	40 duplicate
15101	85 [529; Methyldiictric acid (4 44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	34	0.405	0.724	8,471	0.546	48	94	23	119	42	24 duplicate
8391	85 [529; Methyldiictric acid (4 129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	43	0.404	0.682	9,029	0.408	49	93	35	107	48	112 original
13541	85 [529; Methyldiictric acid (4 29 Erythritol	48	0.401	0.713	2,080	0.525	50	91	24	118	1	36 duplicate
17750	85 [529; Methyldiictric acid (4 76 Fructose	48	0.401	0.590	19,529	0.488	51	92	56	86	116	62 duplicate
8348	85 [529; Methyldiictric acid (4 86 [793; D-Galactono-1,4-lactone (4TMS)]	48	0.399	0.587	16,279	0.487	52	90	57	85	103	63 original



16980	85 [529; Methylcitric acid (4 65 [646; 3-Deoxyglucitol (5TMS)]	47	0.397	0.684	11.978	0.457	53	89	33	109	78	86 duplicate
15282	85 [528; Methylcitric acid (4 46 Arabinose	48	0.395	0.626	11.378	0.450	54	88	47	95	75	92 duplicate
14606	85 [529; Methylcitric acid (4 39 [829; 1-Phenylethanol (1TMS)]	47	0.395	0.731	9.639	0.456	55	87	19	123	56	87 duplicate
8350	85 [528; Methylcitric acid (4 88 Gluconic acid	48	0.394	0.661	5.828	0.528	56	86	41	101	20	34 original
13202	85 [529; Methylcitric acid (4 26 Citramalic acid	48	0.388	0.736	11.968	0.514	57	85	18	124	77	41 duplicate
12007	85 [528; Methylcitric acid (4 16 [644; 2-Methyl-1,3-butanediol (2TMS)]	48	0.385	0.705	11.281	0.506	58	84	28	114	73	50 duplicate
17877	85 [528; Methylcitric acid (4 78 Mannose	47	0.380	0.608	9.443	0.477	59	83	64	88	63	73 duplicate
8368	85 [529; Methylcitric acid (4 106 [733; Threitol (4TMS)]	46	0.372	0.677	8.668	0.540	60	82	35	108	45	26 original
12971	85 [528; Methylcitric acid (4 24 [725; 2-Ketooctanoic acid (2TMS)]	48	0.371	0.690	23.616	0.477	61	81	32	110	122	74 duplicate
8373	85 [528; Methylcitric acid (4 11 [583; Erythritol (4TMS)]	30	0.356	0.572	15.283	0.481	62	80	58	84	95	70 original
12617	85 [529; Methylcitric acid (4 21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	48	0.355	0.670	11.637	0.519	63	79	38	104	76	37 duplicate
8368	85 [528; Methylcitric acid (4 104 [795; Erythritol (4TMS)]	48	0.346	0.519	5.436	0.483	64	78	68	78	17	67 original
17552	85 [528; Methylcitric acid (4 73 [708; Glucose methoxamine (5TMS)]	48	0.337	0.595	8.532	0.456	65	77	55	87	44	88 duplicate
8385	85 [528; Methylcitric acid (4 123 [945; Galactoturanose-6-phosphate (7TMS)]	48	0.333	0.457	7.827	0.468	66	76	70	72	37	78 original
12254	85 [528; Methylcitric acid (4 18 [590; 1-Acetyl-2-thiohydantoin	48	0.332	0.616	4.176	0.438	67	75	50	92	9	98 duplicate
12376	85 [528; Methylcitric acid (4 19 Alanine (BP) (3TMS)	48	0.323	0.524	8.950	0.453	68	74	65	77	46	89 duplicate
8386	124 [734; 1-Monooleoylglycerol (2TMS); 1-Monoheptadecenoylglycerol (1TMS)]	44	0.313	0.326	17.362	0.422	69	73	73	69	107	108 original
14807	85 [528; Methylcitric acid (4 41 [639; Proline (2TMS)]	48	0.301	0.499	10.423	0.421	70	71	68	74	64	108 duplicate
8387	85 [528; Methylcitric acid (4 125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru	48	0.301	0.407	24.886	0.344	71	72	71	71	124	134 original
12131	85 [528; Methylcitric acid (4 17 [700; 2-methyl-1,2-propanediol (2TMS)]	48	0.282	0.561	11.127	0.396	72	70	61	81	72	120 duplicate
8365	85 [528; Methylcitric acid (4 103 [648; Ethylamine (2TMS)]	47	0.254	0.507	7.541	0.462	73	69	67	75	34	81 original
8359	85 [529; Methylcitric acid (4 97 [756; beta-D-Methylglucopyranoside (4TMS)]	36	0.210	0.318	9.048	0.446	74	68	74	68	57	98 original
8401	85 [528; Methylcitric acid (4 139 [700; Ergosta-5,7-dien-3-ol	29	0.192	0.211	14.380	0.328	75	67	83	59	92	135 original
8381	85 [528; Methylcitric acid (4 119 [931; myo-Inositol-2-phosphate (7TMS)]	48	0.158	0.299	5.802	0.446	76	66	76	68	19	95 original
8358	85 [528; Methylcitric acid (4 66 myo-Inositol	41	0.151	0.212	16.093	0.286	77	65	82	60	102	140 original
16590	85 [528; Methylcitric acid (4 90 Glycerol-3-phosphate	48	0.147	0.240	18.504	0.462	78	64	79	63	110	82 duplicate
10712	85 [528; Methylcitric acid (4 6 Glycerol	48	0.137	0.215	34.575	0.307	79	63	81	61	139	139 duplicate
8369	85 [529; Methylcitric acid (4 107 9-(Z)-Octadecenoic acid	48	0.135	0.135	10.991	0.384	80	62	87	55	71	123 original
16904	85 [528; Methylcitric acid (4 64 [789; Tyramine (3TMS)]	47	0.129	0.193	2.796	0.408	81	61	84	58	3	111 duplicate
17129	85 [529; Methylcitric acid (4 67 Citric acid	48	0.094	0.139	19.904	0.475	82	60	86	56	117	75 duplicate
8352	85 [528; Methylcitric acid (4 90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	48	0.092	0.090	4.389	0.360	83	59	90	52	13	129 original
8349	85 [528; Methylcitric acid (4 87 [945; beta-D-Glucopyranose (5TMS)]	48	0.087	0.300	27.867	0.274	84	57	75	67	130	141 original
8363	85 [528; Methylcitric acid (4 101 [832; Dopamine (4TMS)]	48	0.087	0.255	5.625	0.492	85	58	77	65	18	61 original
18234	85 [528; Methylcitric acid (4 84 Mannitol	46	0.078	-0.045	19.100	0.503	86	56	95	47	114	52 duplicate
10846	85 [528; Methylcitric acid (4 7 Threonine	48	0.073	0.072	26.046	0.566	87	55	91	51	128	18 duplicate
11862	85 [528; Methylcitric acid (4 15 Alanine	48	0.064	0.103	15.242	0.437	88	54	89	53	94	99 duplicate
8353	85 [528; Methylcitric acid (4 91 [766; beta-D-Methylglucopyranoside (4TMS)]	48	0.046	0.132	8.489	0.508	89	53	88	54	43	47 original
17839	85 [529; Methylcitric acid (4 79 Glucose	48	0.009	0.241	29.331	0.452	90	52	78	64	135	90 duplicate
18000	85 [528; Methylcitric acid (4 80 [772; D-Glucose (5TMS)]	46	0.001	0.156	24.050	0.349	91	51	85	57	123	132 duplicate
8398	85 [528; Methylcitric acid (4 136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	13	0.000	0.019	2.459	0.353	92	50	93	49	2	131 original
14287	85 [528; Methylcitric acid (4 36 [596; N-Acetylglutamic acid (2TMS)]	42	-0.005	-0.055	26.021	0.568	93	49	98	46	127	15 duplicate
8360	85 [529; Methylcitric acid (4 118 [928; Glucopyranose-6-phosphate (6TMS)]	48	-0.010	0.060	7.467	0.381	94	48	92	50	32	125 original
10027	85 [528; Methylcitric acid (4 1 [838; Sulfuric acid (2TMS)]	20	-0.021	0.220	7.135	0.430	95	47	80	82	29	103 duplicate
8392	85 [528; Methylcitric acid (4 130 Trehalose	47	-0.027	-0.078	25.382	0.407	96	46	97	45	125	114 original
8370	85 [528; Methylcitric acid (4 108 Octadecenoic acid	48	-0.035	-0.089	4.279	0.419	97	45	98	44	11	110 original
14401	85 [528; Methylcitric acid (4 37 Phenylalanine	48	-0.039	-0.120	19.331	0.487	98	44	99	43	115	64 duplicate
8355	85 [528; Methylcitric acid (4 93 [607; Putrescine (4TMS)]	45	-0.061	-0.027	14.143	0.518	99	43	94	48	89	38 original
15929	85 [528; Methylcitric acid (4 53 Glycerol-2-phosphate	48	-0.086	-0.271	8.255	0.378	100	42	105	37	40	127 duplicate
12497	20 [619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.097	-0.515	14.118	0.504	101	41	120	22	88	51 duplicate

16427	85 [529; Methylethyl acid (4	[636; 4R-Acetamide-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane	58	(1TMS)]	48	-0.098	-0.129	13.984	0.589	102	40	100	42	87	6 duplicate
17685	85 [529; Methylethyl acid (4	Lysine	75		48	-0.110	-0.148	35.402	0.566	103	39	101	41	140	17 duplicate
8357	85 [529; Methylethyl acid (4	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	95	[NA]	36	-0.133	-0.277	13.438	0.483	104	38	106	36	86	68 original
17484	85 [529; Methylethyl acid (4	[918; D-Xylopyranose (4TMS)]	72		48	-0.149	-0.167	4.348	0.321	105	36	102	40	12	137 duplicate
10441	85 [529; Methylethyl acid (4	Phosphoric acid	4		48	-0.149	-0.287	7.835	0.380	106	37	108	34	38	128 duplicate
10304	85 [529; Methylethyl acid (4	Ethanolamine	3		47	-0.166	-0.209	31.353	0.405	107	35	103	39	136	115 duplicate
17055	85 [529; Methylethyl acid (4	Glyceric acid-3-phosphate	66		47	-0.177	-0.284	6.480	0.480	108	34	107	35	25	72 duplicate
15386	85 [529; Methylethyl acid (4	[NA]	47		48	-0.211	-0.266	2.957	0.576	109	33	104	38	4	13 duplicate
16509	85 [529; Methylethyl acid (4	Ornithine; Arginine	59		48	-0.215	-0.324	9.044	0.388	110	32	109	33	49	122 duplicate
17814	85 [529; Methylethyl acid (4	[826; beta-[[5-methyl-2-thienyl]methyl]eneamino-benzeneacetic acid methyl ester]	77		48	-0.230	-0.543	36.367	0.537	111	31	127	15	141	27 duplicate
15841	85 [529; Methylethyl acid (4	[NA]	52		48	-0.248	-0.394	28.384	0.525	112	30	111	31	132	35 duplicate
15752	85 [529; Methylethyl acid (4	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	51		30	-0.251	-0.412	15.647	0.500	113	29	112	30	98	54 duplicate
13762	85 [529; Methylethyl acid (4	[622; Parabanic acid (2TMS)]	31		39	-0.258	-0.540	15.323	0.506	114	28	126	16	96	49 duplicate
14906	85 [529; Methylethyl acid (4	Glutamic acid	42		48	-0.268	-0.536	8.361	0.532	115	27	125	17	24	30 duplicate
10979	85 [529; Methylethyl acid (4	Isoleucine	8		47	-0.269	-0.571	28.619	0.580	116	26	128	14	133	9 duplicate
11111	85 [529; Methylethyl acid (4	Proline	9		48	-0.270	-0.436	15.864	0.498	117	24	114	28	98	58 duplicate
15197	85 [529; Methylethyl acid (4	Homocysteine	45		48	-0.270	-0.529	25.844	0.603	118	25	121	21	128	3 duplicate
18060	85 [529; Methylethyl acid (4	Tyrosine	81		45	-0.271	-0.536	16.650	0.450	119	23	124	18	105	91 duplicate
16102	85 [529; Methylethyl acid (4	[812; 4-Aminobutyric acid (2TBS)]	55		48	-0.277	-0.422	31.954	0.549	120	22	113	29	137	21 duplicate
13979	85 [529; Methylethyl acid (4	Methionine	33		42	-0.282	-0.374	19.927	0.383	121	21	110	32	119	124 duplicate
13652	85 [529; Methylethyl acid (4	[815; Ethyl-3(2H)-thiophenone]	30		48	-0.298	-0.465	9.299	0.528	122	20	115	27	52	32 duplicate
10166	85 [529; Methylethyl acid (4	Serine	2		48	-0.307	-0.495	27.312	0.533	123	19	118	24	129	29 duplicate
10577	85 [529; Methylethyl acid (4	Leucine	5		48	-0.309	-0.491	16.354	0.576	124	18	117	25	104	12 duplicate
8393	85 [529; Methylethyl acid (4	[626; 5-Methylthioadenosine (3TMS)]	131		45	-0.313	-0.618	10.380	0.471	125	17	131	11	63	77 duplicate
15479	85 [529; Methylethyl acid (4	Asparagine	48		42	-0.322	-0.672	12.935	0.514	126	16	135	7	83	42 original
15004	85 [529; Methylethyl acid (4	[548; Leucine (2TBS)]	43		48	-0.326	-0.532	11.343	0.461	127	15	122	20	74	83 duplicate
15571	85 [529; Methylethyl acid (4	[877; Pyrophosphoric acid (4TMS)]	49		46	-0.328	-0.534	6.759	0.424	128	14	123	19	27	105 duplicate
17274	85 [529; Methylethyl acid (4	Arginine	69		48	-0.332	-0.643	17.435	0.422	129	13	132	10	108	107 duplicate
11242	85 [529; Methylethyl acid (4	Glycine	10		48	-0.339	-0.653	20.564	0.511	130	12	134	8	121	44 duplicate
13316	85 [529; Methylethyl acid (4	[815; (E)-4-Methyl-5-hydroxy-3-pentan-2-one (1TMS)]	27		48	-0.351	-0.646	17.594	0.468	131	11	133	9	109	78 duplicate
16827	85 [529; Methylethyl acid (4	Glutamine	63		44	-0.353	-0.737	13.432	0.551	132	10	138	4	85	20 duplicate
8360	85 [529; Methylethyl acid (4	[897; Ribose-5-phosphate methoxyamine (5TMS)]	98		36	-0.365	-0.489	14.857	0.313	133	9	116	26	83	138 duplicate
14086	85 [529; Methylethyl acid (4	Aspartic acid	34		35	-0.368	-0.692	12.611	0.625	134	8	136	6	80	1 original
12854	85 [529; Methylethyl acid (4	Homoserine	23		48	-0.376	-0.507	28.916	0.497	135	7	119	23	134	57 duplicate
13087	85 [529; Methylethyl acid (4	[709; 2,5-Diaminovalerolactam (2TMS)]	25		48	-0.383	-0.771	10.361	0.578	136	6	140	2	62	11 duplicate
13871	85 [529; Methylethyl acid (4	Lysine	82		32	-0.395	-0.775	12.712	0.568	137	5	141	1	82	16 duplicate
18119	85 [529; Methylethyl acid (4	[775; Dopamine (4TMS)]	89		48	-0.404	-0.610	9.483	0.613	138	4	130	12	54	2 duplicate
8351	85 [529; Methylethyl acid (4	[570; Hypoxanthine (2TMS)]	68		39	-0.441	-0.710	16.726	0.435	139	3	137	5	108	100 duplicate
17202	85 [529; Methylethyl acid (4	Arabinose	46		30	-0.457	-0.589	15.428	0.458	140	2	129	13	97	85 original
15293	86 [793; D-Galactono-1,4-l	[829; Orolic acid (3TMS)]	56		16	-0.533	-0.753	10.605	0.426	141	1	139	3	65	104 duplicate
16281	86 [793; D-Galactono-1,4-l	[829; Orolic acid (3TMS)]	56		61	0.858	0.991	5.924	0.719	1	141	1	141	1	4 duplicate
16981	86 [793; D-Galactono-1,4-l	[846; 3-Deoxyglucitol (5TMS)]	65		61	0.849	0.985	17.214	0.711	2	140	3	139	32	8 duplicate
16345	86 [793; D-Galactono-1,4-l	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	57		60	0.847	0.979	16.081	0.715	3	139	5	137	24	6 duplicate
12972	86 [793; D-Galactono-1,4-l	[725; 2-Ketooctanoic acid (2TMS)]	26		52	0.845	0.988	11.629	0.687	4	138	2	140	6	15 duplicate
12008	86 [793; D-Galactono-1,4-l	[844; 2-Methyl-1,3-butanediol (2TMS)]	14		61	0.837	0.960	20.930	0.726	5	137	7	135	56	2 duplicate
8451	86 [793; D-Galactono-1,4-l	Isomaltose	134		61	0.820	0.935	13.684	0.725	6	136	12	130	12	3 duplicate
15663	86 [793; D-Galactono-1,4-l	[746; Ribonic acid-1,4-lactone (3TMS)]	50		61	0.807	0.980	9.365	0.726	7	135	4	138	3	1 original
					58	0.806	0.901	31.207	0.617	8	134	21	121	123	47 duplicate

11630	86 [793; D-Galactono-1,4-di	129	Uracil	61	0.800	0.943	11.303	0.703	9	133	11	131	5	10 duplicate
8446	86 [793; D-Galactono-1,4-di	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	56	0.786	0.958	15.167	0.686	10	132	8	134	14	16 original
14607	86 [793; D-Galactono-1,4-di	39	[829; 1-Phenylethanol (1TMS)]	60	0.784	0.925	9.087	0.675	11	131	15	127	2	18 duplicate
8405	86 [793; D-Galactono-1,4-di	88	Gluconic acid	61	0.775	0.909	12.818	0.678	12	130	19	123	9	18 original
13542	86 [793; D-Galactono-1,4-di	29	Erythritol	61	0.774	0.891	20.335	0.635	13	129	24	118	53	40 duplicate
16750	86 [793; D-Galactono-1,4-di	62	[812; D-Xylofuranose (4TMS)]	61	0.766	0.949	15.602	0.669	14	128	10	132	19	24 duplicate
12132	86 [793; D-Galactono-1,4-di	17	[700; 2-methyl-1,2-propanediol (2TMS)]	61	0.760	0.917	12.583	0.594	15	127	17	125	7	60 duplicate
14505	86 [793; D-Galactono-1,4-di	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	61	0.751	0.916	17.078	0.672	16	126	18	124	29	22 duplicate
17553	86 [793; D-Galactono-1,4-di	73	[708; 2,3-Dimethylsuccinic acid (2TMS)]	55	0.721	0.865	15.806	0.564	17	125	29	113	21	70 duplicate
16017	86 [793; D-Galactono-1,4-di	54	[NA]	52	0.710	0.932	22.975	0.610	18	124	14	128	73	51 duplicate
11373	86 [793; D-Galactono-1,4-di	11	Succinic acid	61	0.684	0.893	17.655	0.624	19	123	23	119	36	44 duplicate
17878	86 [793; D-Galactono-1,4-di	78	Mannose	59	0.677	0.885	18.499	0.602	20	122	25	117	42	57 duplicate
17751	86 [793; D-Galactono-1,4-di	76	Fructose	61	0.677	0.965	12.746	0.695	21	121	6	136	8	13 duplicate
11757	86 [793; D-Galactono-1,4-di	14	Fumaric acid	61	0.666	0.882	23.376	0.630	22	120	28	118	79	42 duplicate
8423	86 [793; D-Galactono-1,4-di	106	[733; Threitol (4TMS)]	59	0.658	0.908	13.446	0.719	23	119	20	122	11	5 original
8442	86 [793; D-Galactono-1,4-di	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	61	0.654	0.921	19.106	0.616	24	118	18	126	45	48 original
14708	86 [793; D-Galactono-1,4-di	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	61	0.650	0.852	27.196	0.630	25	117	34	108	98	43 duplicate
13430	86 [793; D-Galactono-1,4-di	28	Malic acid	61	0.639	0.880	17.197	0.661	26	116	27	115	30	26 duplicate
14193	86 [793; D-Galactono-1,4-di	35	Pyroglutamic acid	61	0.619	0.949	30.866	0.678	27	115	9	133	120	17 duplicate
8416	86 [793; D-Galactono-1,4-di	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	38	0.616	0.857	22.924	0.637	28	114	33	109	72	38 original
8420	86 [793; D-Galactono-1,4-di	103	[648; Ethylamine (2TMS)]	60	0.614	0.795	14.235	0.579	29	113	43	99	13	64 original
12737	86 [793; D-Galactono-1,4-di	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	51	0.605	0.838	23.891	0.648	30	112	36	106	81	32 duplicate
11502	86 [793; D-Galactono-1,4-di	12	Glyceric acid	60	0.601	0.764	25.147	0.582	31	111	44	98	86	63 duplicate
8409	86 [793; D-Galactono-1,4-di	92	[680; Glycerol-2-phosphate (4TMS)]	51	0.600	0.894	17.941	0.605	32	110	22	120	38	54 original
8432	86 [793; D-Galactono-1,4-di	115	Glucose-6-phosphate	59	0.592	0.933	15.558	0.665	33	109	13	129	18	25 original
12618	86 [793; D-Galactono-1,4-di	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	61	0.563	0.749	16.351	0.584	34	108	49	93	26	71 duplicate
8438	86 [793; D-Galactono-1,4-di	121	[657; Erythritol (4TMS)]	52	0.540	0.780	26.390	0.647	35	107	46	96	92	34 original
10713	86 [793; D-Galactono-1,4-di	6	Glycerol	61	0.540	0.836	32.009	0.566	36	106	37	105	127	69 duplicate
8427	86 [793; D-Galactono-1,4-di	110	[715; Erythritol (4TMS)]	51	0.537	0.873	20.552	0.695	37	105	28	114	54	14 original
17346	86 [793; D-Galactono-1,4-di	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	54	0.529	0.671	15.435	0.517	38	104	56	86	16	93 duplicate
13203	86 [793; D-Galactono-1,4-di	26	Citramalic acid	61	0.527	0.779	17.890	0.550	39	103	47	95	37	76 duplicate
8439	86 [793; D-Galactono-1,4-di	117	[644; Erythritol (4TMS)]	49	0.522	0.849	26.899	0.641	40	102	35	107	95	36 original
8434	86 [793; D-Galactono-1,4-di	105	[705; 2-Ketogluconic acid (5TMS)]	53	0.517	0.783	18.828	0.641	41	101	45	97	44	37 original
8414	86 [793; D-Galactono-1,4-di	97	[756; beta-D-Methylglucopyranoside (4TMS)]	45	0.507	0.834	15.805	0.643	43	99	39	103	20	35 original
8404	86 [793; D-Galactono-1,4-di	87	[945; beta-D-Glucopyranose (5TMS)]	59	0.488	0.835	22.705	0.535	45	97	38	104	69	65 original
8418	86 [793; D-Galactono-1,4-di	101	[832; Dopamine (4TMS)]	61	0.484	0.894	17.269	0.531	46	96	52	90	33	85 original
8408	86 [793; D-Galactono-1,4-di	91	[766; beta-D-Methylglucopyranoside (4TMS)]	61	0.479	0.836	17.627	0.494	47	95	61	81	35	111 original
15102	86 [793; D-Galactono-1,4-di	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	47	0.478	0.821	15.977	0.655	48	94	40	102	22	28 duplicate
8437	86 [793; D-Galactono-1,4-di	120	[945; Uridine (3TMS)]	51	0.478	0.923	16.001	0.631	49	93	72	70	23	41 original
8445	86 [793; D-Galactono-1,4-di	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	42	0.461	0.865	15.449	0.651	50	92	30	112	17	30 original
8417	86 [793; D-Galactono-1,4-di	100	[857; Mannitol (6TMS)]	61	0.458	0.863	18.104	0.555	51	91	57	85	39	75 original
8419	86 [793; D-Galactono-1,4-di	102	[904; Galactose methoxyamine (5TMS)]	61	0.456	0.818	22.120	0.559	52	90	62	80	66	73 original
8430	86 [793; D-Galactono-1,4-di	113	Galactose-6-phosphate	59	0.419	0.859	19.801	0.593	53	89	32	110	49	68 original
8421	86 [793; D-Galactono-1,4-di	104	[795; Erythritol (4TMS)]	60	0.412	0.877	16.279	0.487	54	88	55	87	40	108 duplicate
18291	86 [793; D-Galactono-1,4-di	85	[529; Methylcitric acid (4TMS)]	48	0.399	0.587	16.279	0.487	55	87	65	77	25	109 duplicate
8429	86 [793; D-Galactono-1,4-di	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (8TMS)]	60	0.392	0.639	30.835	0.544	56	86	60	82	118	79 original
12255	86 [793; D-Galactono-1,4-di	18	[590; 1-Acetyl-2-thiohydantoin]	61	0.388	0.598	18.763	0.468	57	85	63	79	43	116 duplicate
8449	86 [793; D-Galactono-1,4-di	132	[895; Isomaltose methoxyamine (8TMS)]	39	0.379	0.861	25.471	0.659	58	84	31	111	90	27 original
12377	86 [793; D-Galactono-1,4-di	19	Alanine [BP] (3TMS)	61	0.375	0.758	15.176	0.558	59	83	48	94	15	74 duplicate

8443	86 [793; D-Galactono-1,4-di	126	[559; Erythritol (4TMS)]	42	0.368	0.685	21,476	0.698	60	82	54	88	61	11 original
17620	86 [793; D-Galactono-1,4-di	74	[912; Tetradecanoic acid (1TMS)]	61	0.353	0.594	18,983	0.504	61	81	64	78	51	100 duplicate
8452	86 [793; D-Galactono-1,4-di	135	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	61	0.352	0.507	18,452	0.540	62	80	69	73	41	80 original
10028	86 [793; D-Galactono-1,4-di	1	[938; Sulfuric acid (2TMS)]	33	0.348	0.585	21,093	0.619	63	79	66	76	58	48 duplicate
8431	86 [793; D-Galactono-1,4-di	114	Fructose-6-phosphate	50	0.324	0.816	21,031	0.808	64	78	41	101	57	52 original
8444	86 [793; D-Galactono-1,4-di	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	36	0.321	0.689	19,224	0.696	65	77	53	89	47	12 original
14808	86 [793; D-Galactono-1,4-di	41	[639; Proline (2TMS)]	61	0.295	0.582	16,688	0.472	66	76	67	75	27	113 duplicate
18001	86 [793; D-Galactono-1,4-di	80	[772; D-Glucose (5TMS)]	59	0.290	0.740	20,045	0.501	67	75	51	91	52	101 duplicate
8440	86 [793; D-Galactono-1,4-di	123	[945; Galactofuranose-6-phosphate (7TMS)]	61	0.281	0.648	17,189	0.574	68	74	59	83	31	67 original
18178	86 [793; D-Galactono-1,4-di	83	Sorbitol	55	0.271	-0.189	22,860	0.378	69	73	90	52	71	136 duplicate
17940	86 [793; D-Galactono-1,4-di	79	Glucose	61	0.223	0.740	24,925	0.612	70	72	50	92	85	50 duplicate
8433	86 [793; D-Galactono-1,4-di	116	[892; Pseudouridine (5TMS)]	30	0.172	0.229	17,576	0.512	71	71	77	65	34	85 original
16905	86 [793; D-Galactono-1,4-di	64	[789; Tyramine (3TMS)]	60	0.160	0.441	21,776	0.486	72	70	70	72	63	110 duplicate
11893	86 [793; D-Galactono-1,4-di	15	Alanine	61	0.151	0.539	16,796	0.670	73	69	68	74	28	23 duplicate
8450	86 [793; D-Galactono-1,4-di	133	[855; Squalene]	61	0.138	0.105	21,541	0.384	74	68	80	62	62	135 original
8413	86 [793; D-Galactono-1,4-di	96	myo-Inositol	47	0.130	0.209	29,956	0.328	75	67	78	64	111	141 original
18235	86 [793; D-Galactono-1,4-di	84	Mannitol	59	0.127	0.321	24,431	0.466	76	66	73	69	83	118 duplicate
15387	86 [793; D-Galactono-1,4-di	47	[NA]	61	0.104	0.168	22,664	0.451	77	65	79	63	68	125 duplicate
8426	86 [793; D-Galactono-1,4-di	109	Octadecanoic acid	61	0.104	0.394	19,209	0.535	78	64	71	71	46	82 original
8428	86 [793; D-Galactono-1,4-di	111	[583; Erythritol (4TMS)]	40	0.085	0.291	33,823	0.473	79	63	74	68	130	112 original
8410	86 [793; D-Galactono-1,4-di	93	[607; Putrescine (4TMS)]	57	0.075	0.092	31,036	0.468	80	62	83	59	122	117 original
15930	86 [793; D-Galactono-1,4-di	53	Glycerol-2-phosphate	61	0.052	-0.129	27,347	0.358	81	61	85	57	98	137 duplicate
8457	86 [793; D-Galactono-1,4-di	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	48	0.037	0.092	28,352	0.497	82	60	82	60	103	102 original
8411	86 [793; D-Galactono-1,4-di	94	Hexadecanoic acid	61	0.031	0.275	19,881	0.517	83	59	76	66	50	92 original
8407	86 [793; D-Galactono-1,4-di	80	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	61	-0.002	-0.181	22,077	0.436	84	58	88	54	65	131 original
8458	86 [793; D-Galactono-1,4-di	141	Lanosta-8,24-dien-3-beta-ol	59	-0.020	-0.047	28,683	0.519	85	57	84	58	105	89 original
8455	86 [793; D-Galactono-1,4-di	138	[674; Ergosterol (1TMS)]	44	-0.025	0.097	29,031	0.511	86	56	81	61	107	96 original
8435	86 [793; D-Galactono-1,4-di	118	[928; Glucopyranose-6-phosphate (8TMS)]	55	-0.061	0.289	23,017	0.447	87	55	75	67	75	126 original
8454	86 [793; D-Galactono-1,4-di	137	Ergosterol	61	-0.080	-0.186	22,067	0.518	88	54	89	53	64	90 original
8424	86 [793; D-Galactono-1,4-di	107	9-(Z)-Octadecenoic acid	61	-0.104	-0.386	20,628	0.464	89	53	99	43	55	119 original
17416	86 [793; D-Galactono-1,4-di	71	[731; Erythrose (3TMS)]	61	-0.113	-0.178	19,647	0.492	90	52	87	55	48	105 duplicate
8456	86 [793; D-Galactono-1,4-di	139	[700; Ergosta-5,7-dien-3-ol]	37	-0.114	-0.200	30,462	0.495	91	51	91	51	113	103 original
16828	86 [793; D-Galactono-1,4-di	63	Glutamine	49	-0.122	-0.814	34,647	0.707	92	50	128	14	134	9 duplicate
8436	86 [793; D-Galactono-1,4-di	119	[931; myo-Inositol-2-phosphate (7TMS)]	61	-0.143	-0.307	23,331	0.562	93	49	95	47	78	72 original
17485	86 [793; D-Galactono-1,4-di	72	[919; D-Xylopyranose (4TMS)]	60	-0.147	-0.157	25,305	0.329	94	48	86	56	87	140 duplicate
8447	86 [793; D-Galactono-1,4-di	130	Trehalose	60	-0.154	-0.223	25,372	0.429	95	47	92	50	89	134 original
10442	86 [793; D-Galactono-1,4-di	4	Phosphoric acid	49	-0.163	-0.293	30,235	0.352	96	46	93	49	112	139 duplicate
8441	86 [793; D-Galactono-1,4-di	124	[734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecenoylethanol (1TMS)]	56	-0.170	-0.372	37,159	0.439	97	45	98	44	139	128 original
15005	86 [793; D-Galactono-1,4-di	43	[548; Leucine (2TBS)]	58	-0.204	-0.365	22,283	0.464	98	44	96	46	67	120 duplicate
86 [793; D-Galactono-1,4-di	58	[636; 4R-Acetamidido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	61	-0.207	-0.300	21,439	0.432	99	43	94	48	59	133 duplicate	
16428	86 [793; D-Galactono-1,4-di	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	16	-0.250	-0.370	13,330	0.545	100	42	97	45	10	78 original
8453	86 [793; D-Galactono-1,4-di	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	45	-0.261	-0.703	30,773	0.594	101	41	118	24	116	61 original
8415	86 [793; D-Galactono-1,4-di	52	[NA]	43	-0.287	-0.767	34,664	0.674	102	40	125	17	135	20 duplicate
15842	86 [793; D-Galactono-1,4-di	36	[596; N-Acetylglutamic acid (2TMS)]	61	-0.289	-0.469	27,208	0.438	103	39	102	40	97	130 duplicate
14298	86 [793; D-Galactono-1,4-di	75	Lysine	61	-0.294	-0.420	34,017	0.454	104	38	100	42	131	122 duplicate
13317	86 [793; D-Galactono-1,4-di	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	-0.299	-0.714	34,558	0.546	105	37	119	23	132	77 duplicate
8425	86 [793; D-Galactono-1,4-di	108	Octadecanoic acid	61	-0.326	-0.554	25,347	0.435	106	36	106	36	88	132 original
16671	86 [793; D-Galactono-1,4-di	61	[NA]	61	-0.343	-0.554	23,636	0.520	107	35	107	35	80	87 duplicate

10847	86 [793; D-Galactono-1,4-l	7	Threonine	61	-0.348	-0.486	28.581	0.469	108	34	103	39	93	115 duplicate
13088	86 [793; D-Galactono-1,4-l	25	[709; 2,5-Diaminovalerolactam (2TMS)]	45	-0.354	-0.865	31.608	0.821	109	33	133	9	125	45 duplicate
12855	86 [793; D-Galactono-1,4-l	23	Homoserine	61	-0.358	-0.765	27.679	0.598	110	32	124	18	100	59 duplicate
17056	86 [793; D-Galactono-1,4-l	68	Glyceric acid-3-phosphate	61	-0.360	-0.519	24.626	0.510	111	31	104	38	84	98 duplicate
10187	86 [793; D-Galactono-1,4-l	2	Serine	60	-0.395	-0.530	28.037	0.439	112	30	105	37	101	128 duplicate
17203	86 [793; D-Galactono-1,4-l	68	[570; Hypoxanthine (2TMS)]	20	-0.432	-0.927	21.469	0.603	113	29	138	4	60	58 duplicate
13763	86 [793; D-Galactono-1,4-l	31	[622; Parabenic acid (2TMS)]	61	-0.433	-0.644	28.701	0.519	114	28	113	29	108	88 duplicate
17130	86 [793; D-Galactono-1,4-l	67	Citric acid	61	-0.435	-0.679	22.829	0.489	115	27	115	27	70	107 duplicate
8406	86 [793; D-Galactono-1,4-l	89	[775; Dopamine (4TMS)]	35	-0.439	-0.917	30.837	0.614	116	26	136	6	119	49 original
10980	86 [793; D-Galactono-1,4-l	8	Isoleucine	54	-0.440	-0.468	26.246	0.355	117	25	101	41	91	138 duplicate
15572	86 [793; D-Galactono-1,4-l	49	[877; Pyrophosphoric acid (4TMS)]	61	-0.445	-0.638	37.685	0.490	118	24	112	30	141	106 duplicate
16591	86 [793; D-Galactono-1,4-l	60	Glycerol-3-phosphate	61	-0.450	-0.616	23.057	0.508	119	23	109	33	77	99 duplicate
15198	86 [793; D-Galactono-1,4-l	45	Homocysteine	58	-0.483	-0.627	35.992	0.461	120	22	111	31	138	121 duplicate
14402	86 [793; D-Galactono-1,4-l	37	Phenylalanine	61	-0.490	-0.683	22.996	0.471	121	21	116	26	74	114 duplicate
11112	86 [793; D-Galactono-1,4-l	9	Proline	60	-0.494	-0.597	31.669	0.452	122	20	108	34	126	124 duplicate
14087	86 [793; D-Galactono-1,4-l	34	Aspartic acid	61	-0.508	-0.625	30.510	0.518	123	19	110	32	114	91 duplicate
8448	86 [793; D-Galactono-1,4-l	131	[626; 5-Methylthioadenosine (3TMS)]	52	-0.508	-0.754	30.796	0.607	124	18	121	21	117	53 original
15480	86 [793; D-Galactono-1,4-l	48	Asparagine	61	-0.516	-0.667	29.921	0.650	125	17	134	8	110	31 duplicate
13980	86 [793; D-Galactono-1,4-l	33	Methionine	61	-0.565	-0.668	27.413	0.523	126	16	114	28	99	86 duplicate
8412	86 [793; D-Galactono-1,4-l	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	47	-0.582	-0.816	31.456	0.532	127	15	129	13	124	83 original
15753	86 [793; D-Galactono-1,4-l	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	42	-0.584	-0.779	28.091	0.532	128	14	127	15	102	84 duplicate
16510	86 [793; D-Galactono-1,4-l	59	Ornithine; Arginine	61	-0.595	-0.725	35.857	0.510	129	13	120	22	137	97 duplicate
10305	86 [793; D-Galactono-1,4-l	3	Ethanolamine	59	-0.612	-0.864	29.523	0.605	130	12	132	10	108	55 duplicate
13653	86 [793; D-Galactono-1,4-l	30	[815; Ethyl-3-(2H)-thiophenone]	61	-0.614	-0.697	30.722	0.452	131	11	117	25	115	123 duplicate
17275	86 [793; D-Galactono-1,4-l	68	Arginine	59	-0.624	-0.854	29.578	0.636	132	10	131	11	109	39 duplicate
16103	86 [793; D-Galactono-1,4-l	55	[612; 4-Aminobutyric acid (2TBS)]	40	-0.631	-0.924	31.029	0.576	133	9	137	5	121	66 duplicate
13872	86 [793; D-Galactono-1,4-l	32	[728; N,N-Dimethyllysine methyl ester]	62	-0.644	-0.771	33.651	0.599	134	8	126	16	129	58 duplicate
10578	86 [793; D-Galactono-1,4-l	5	Leucine	45	-0.661	-0.757	24.371	0.514	135	7	122	20	82	94 duplicate
18120	86 [793; D-Galactono-1,4-l	82	Lysine	39	-0.665	-0.962	28.486	0.673	136	6	140	2	104	21 duplicate
12498	86 [793; D-Galactono-1,4-l	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.677	-0.970	23.022	0.648	137	5	141	1	76	33 duplicate
17815	86 [793; D-Galactono-1,4-l	77	benzeneacetic acid methyl ester	59	-0.681	-0.820	33.209	0.489	138	4	130	12	128	108 duplicate
18061	86 [793; D-Galactono-1,4-l	81	Tyrosine	61	-0.691	-0.898	34.678	0.654	139	3	135	7	136	29 duplicate
11243	86 [793; D-Galactono-1,4-l	10	Glycine	61	-0.706	-0.949	26.872	0.712	140	2	139	3	94	7 duplicate
14907	86 [793; D-Galactono-1,4-l	42	Glutamic acid	58	-0.725	-0.764	34.641	0.493	141	1	123	19	133	104 duplicate
18002	87 [945; beta-D-Glucopyran	80	[772; D-Glucose (5TMS)]	60	0.718	0.960	6.117	0.587	1	141	1	141	1	4 duplicate
11631	87 [945; beta-D-Glucopyran	13	Uracil	62	0.497	0.720	21.828	0.508	2	140	21	121	32	42 duplicate
18347	87 [945; beta-D-Glucopyran	86	[793; D-Galactono-1,4-lactone (4TMS)]	59	0.488	0.835	22.705	0.535	3	139	4	138	36	33 duplicate
15294	87 [945; beta-D-Glucopyran	48	Arabinose	62	0.481	0.813	25.200	0.560	4	138	6	138	45	18 duplicate
16982	87 [945; beta-D-Glucopyran	65	[646; 3-Deoxyglucitol (5TMS)]	61	0.471	0.761	35.821	0.577	5	137	12	130	100	11 duplicate
8505	87 [945; beta-D-Glucopyran	134	Isomaltose	62	0.470	0.787	15.549	0.545	6	136	9	133	13	25 original
8459	87 [945; beta-D-Glucopyran	88	Gluconic acid	62	0.461	0.720	27.372	0.500	7	134	22	120	56	45 original
8472	87 [945; beta-D-Glucopyran	101	[832; Dopamine (4TMS)]	62	0.461	0.594	31.424	0.431	8	135	45	97	74	88 original
16262	87 [945; beta-D-Glucopyran	56	[829; Orolic acid (3TMS)]	59	0.453	0.791	35.990	0.550	9	133	7	135	101	21 duplicate
15664	87 [945; beta-D-Glucopyran	50	[746; Ribonic acid-1,4-lactone (3TMS)]	62	0.447	0.689	48.268	0.463	10	132	26	116	137	61 duplicate
12973	87 [945; beta-D-Glucopyran	24	[725; 2-Keitoclanic acid (2TMS)]	62	0.446	0.730	9.187	0.545	11	131	19	123	4	23 duplicate
8474	87 [945; beta-D-Glucopyran	103	[648; Ethylamine (2TMS)]	61	0.438	0.611	29.984	0.461	12	130	40	102	67	63 original
12133	87 [945; beta-D-Glucopyran	17	[700; 2-methyl-1,2-propanediol (2TMS)]	62	0.435	0.696	20.163	0.502	13	128	24	118	28	44 duplicate
12009	87 [945; beta-D-Glucopyran	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	60	0.435	0.676	19.713	0.508	14	129	29	113	24	43 duplicate
8477	87 [945; beta-D-Glucopyran	108	[733; Threitol (4TMS)]	60	0.434	0.744	28.808	0.529	15	127	16	126	62	35 original

14608	87 [945; beta-D-Glucopyrar 39 [829; 1-Phenylethanol (1TMS)]	61	0.431	0.658	25,000	0.477	16	128	32	110	44	57 duplicate
8500	87 [945; beta-D-Glucopyrar 129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	57	0.429	0.741	32,603	0.585	17	125	17	125	79	8 original
16751	87 [945; beta-D-Glucopyrar 62 [812; D-Xylofuranose (4TMS)]	62	0.414	0.746	22,945	0.500	18	124	15	127	37	46 duplicate
8462	87 [945; beta-D-Glucopyrar 91 [766; beta-D-Methylglucopyranoside (4TMS)]	62	0.401	0.528	32,219	0.421	19	123	55	87	76	92 original
14809	87 [945; beta-D-Glucopyrar 41 [639; Proline (2TMS)]	62	0.399	0.673	23,445	0.500	20	122	31	111	38	47 duplicate
12378	87 [945; beta-D-Glucopyrar 19 Alanine (BP) (3TMS)	62	0.398	0.769	25,351	0.523	21	121	11	131	46	38 duplicate
16018	87 [945; beta-D-Glucopyrar 54 [NA]	53	0.382	0.686	40,121	0.565	22	120	27	115	113	16 duplicate
10714	87 [945; beta-D-Glucopyrar 6 Glyceral	62	0.381	0.770	12,527	0.497	23	119	10	132	7	50 duplicate
17554	87 [945; beta-D-Glucopyrar 73 [708; Glucose methoxyamine (5TMS)]	55	0.380	0.677	32,787	0.456	24	118	28	114	82	69 duplicate
8489	87 [945; beta-D-Glucopyrar 118 [928; Glucopyranose-6-phosphate (6TMS)]	56	0.379	0.686	34,978	0.493	25	117	25	117	97	51 original
8498	87 [945; beta-D-Glucopyrar 125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	62	0.375	0.859	7,491	0.522	26	116	2	140	2	37 original
13543	87 [945; beta-D-Glucopyrar 29 Erythritol	62	0.373	0.587	34,024	0.458	27	115	47	95	89	65 duplicate
16346	87 [945; beta-D-Glucopyrar 57 [757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	53	0.366	0.751	29,723	0.572	28	114	14	128	66	13 duplicate
15388	87 [945; beta-D-Glucopyrar 47 [NA]	62	0.358	0.503	33,108	0.459	29	113	57	85	84	64 duplicate
12738	87 [945; beta-D-Glucopyrar 22 [690; N,N-Di-(2-Hydroxyethyl)-methoxyamine (2TMS)]	50	0.355	0.581	38,540	0.442	30	112	48	94	109	76 duplicate
14508	87 [945; beta-D-Glucopyrar 38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	62	0.354	0.634	30,329	0.458	31	111	36	106	69	68 duplicate
11374	87 [945; beta-D-Glucopyrar 11 Succinic acid	62	0.352	0.809	30,079	0.447	32	110	42	100	68	72 duplicate
13204	87 [945; beta-D-Glucopyrar 26 Citramalic acid	62	0.350	0.563	21,371	0.462	33	109	51	91	31	62 duplicate
17879	87 [945; beta-D-Glucopyrar 78 Mannose	60	0.348	0.719	38,141	0.480	34	108	23	119	102	55 duplicate
11758	87 [945; beta-D-Glucopyrar 14 Fumaric acid	62	0.345	0.614	38,962	0.445	35	107	38	104	110	73 duplicate
8470	87 [945; beta-D-Glucopyrar 99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	39	0.339	0.613	34,466	0.551	36	106	39	103	91	19 original
10029	87 [945; beta-D-Glucopyrar 1 [938; Sulfuric acid (2TMS)]	34	0.337	0.633	30,342	0.628	37	105	37	105	70	1 duplicate
17752	87 [945; beta-D-Glucopyrar 76 Fructose	62	0.333	0.824	12,833	0.538	38	104	5	137	9	31 duplicate
14709	87 [945; beta-D-Glucopyrar 40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	62	0.322	0.567	11,738	0.444	39	103	49	83	5	74 duplicate
12619	87 [945; beta-D-Glucopyrar 21 [678; N,N-Di-(2-Hydroxyethyl)-methoxyamine (2TMS)]	62	0.321	0.501	21,137	0.424	40	102	58	84	30	91 duplicate
17347	87 [945; beta-D-Glucopyrar 70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	55	0.317	0.597	17,100	0.449	41	101	44	88	16	71 duplicate
8468	87 [945; beta-D-Glucopyrar 97 [756; beta-D-Methylglucopyranoside (4TMS)]	50	0.295	0.646	22,479	0.587	42	100	33	109	35	6 original
13431	87 [945; beta-D-Glucopyrar 28 Malic acid	62	0.291	0.594	28,219	0.478	43	99	46	86	59	56 duplicate
8463	87 [945; beta-D-Glucopyrar 92 [680; Glyceral-2-phosphate (4TMS)]	52	0.288	0.649	33,145	0.570	44	98	3	139	85	14 original
8488	87 [945; beta-D-Glucopyrar 117 [724; Glyceral (3TMS)]	54	0.284	0.558	33,598	0.482	45	97	52	90	87	54 original
8486	87 [945; beta-D-Glucopyrar 121 [657; Erythritol (4TMS)]	53	0.279	0.564	41,820	0.514	46	96	50	92	122	41 original
14194	87 [945; beta-D-Glucopyrar 115 Glucose-6-phosphate	60	0.276	0.760	12,699	0.545	47	95	13	129	8	26 original
8475	87 [945; beta-D-Glucopyrar 35 Pyrogulamic acid	62	0.267	0.788	11,746	0.538	48	94	8	134	6	32 duplicate
11503	87 [945; beta-D-Glucopyrar 12 Glycemic acid	62	0.266	0.554	32,706	0.472	49	93	53	89	81	59 original
8491	87 [945; beta-D-Glucopyrar 120 [945; Uridine (3TMS)]	61	0.242	0.446	41,288	0.420	50	92	59	83	119	95 duplicate
8481	87 [945; beta-D-Glucopyrar 110 [715; Erythritol (4TMS)]	52	0.240	0.191	24,542	0.466	51	91	74	68	40	60 original
17941	87 [945; beta-D-Glucopyrar 79 Glucose	62	0.223	0.642	36,980	0.560	52	90	34	108	108	9 original
17486	87 [945; beta-D-Glucopyrar 72 [919; D-Xylopyranose (4TMS)]	61	0.219	0.734	8,692	0.540	53	89	18	124	3	30 duplicate
8494	87 [945; beta-D-Glucopyrar 123 [945; Galactofuranose-6-phosphate (7TMS)]	62	0.211	0.233	36,559	0.377	54	88	71	71	104	118 duplicate
8498	87 [945; beta-D-Glucopyrar 127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	37	0.204	0.525	29,124	0.597	55	87	35	107	55	49 original
12256	87 [945; beta-D-Glucopyrar 18 [590; 1-Acetyl-2-thiohydantoin]	62	0.204	0.365	30,486	0.378	56	84	62	80	71	117 duplicate
8485	87 [945; beta-D-Glucopyrar 114 Fructose-6-phosphate	51	0.200	0.673	33,829	0.561	59	82	30	112	88	17 original
8493	87 [945; beta-D-Glucopyrar 122 [644; Erythritol (4TMS)]	50	0.200	0.540	43,075	0.540	60	83	54	88	125	28 original
8484	87 [945; beta-D-Glucopyrar 113 Galactose-6-phosphate	60	0.198	0.726	35,605	0.568	61	81	20	122	98	15 original
8503	87 [945; beta-D-Glucopyrar 132 [895; Isomaltose methoxyamine (8TMS)]	40	0.195	0.610	39,029	0.549	62	80	41	101	111	22 original
11884	87 [945; beta-D-Glucopyrar 15 Alanine	62	0.193	0.606	19,452	0.516	63	79	43	99	23	40 duplicate
8476	87 [945; beta-D-Glucopyrar 105 [705; 2-Ketogluconic acid (5TMS)]	46	0.173	0.341	30,524	0.597	64	78	66	76	72	2 original
8467	87 [945; beta-D-Glucopyrar 96 myo-Inositol	47	0.169	0.158	44,151	0.304	65	77	77	65	129	138 original

8483	87 [945; beta-D-Glucopyran 112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	61	0.167	0.341	46,793	0.425	66	76	67	75	138	89 original
8489	87 [945; beta-D-Glucopyran 128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	43	0.165	0.437	28,846	0.577	67	75	60	82	63	12 original
17621	87 [945; beta-D-Glucopyran 74 [912; Tetradecanoic acid (1TMS)]	62	0.134	0.361	35,700	0.388	68	74	63	79	99	110 duplicate
8507	87 [945; beta-D-Glucopyran 136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	16	0.133	0.360	18,498	0.517	69	73	64	78	22	39 original
8471	87 [945; beta-D-Glucopyran 100 [857; Mannitol (6TMS)]	62	0.120	0.268	29,294	0.432	70	72	70	72	65	85 original
15103	87 [945; beta-D-Glucopyran 44 [910; 2-Ketogluconic acid methoxamine (4TMS)]	48	0.101	0.357	31,837	0.588	71	71	65	77	75	3 duplicate
8473	87 [945; beta-D-Glucopyran 102 [904; Galactose methoxamine (5TMS)]	62	0.099	0.190	36,351	0.442	72	70	75	67	103	75 original
8487	87 [945; beta-D-Glucopyran 116 [892; Pseudouridine (5TMS)]	30	0.090	-0.027	26,400	0.313	73	69	85	67	54	138 original
18282	87 [945; beta-D-Glucopyran 85 [529; Methylcitic acid (4TMS)]	48	0.087	0.300	27,887	0.274	74	68	69	73	58	141 duplicate
16806	87 [945; beta-D-Glucopyran 64 [788; Tyramine (3TMS)]	61	0.056	0.303	34,582	0.418	75	67	68	74	94	98 duplicate
8506	87 [945; beta-D-Glucopyran [902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	62	0.044	0.152	25,592	0.420	76	68	78	64	49	94 original
8504	87 [945; beta-D-Glucopyran 133 [855; Squalene]	62	0.038	0.077	32,814	0.374	77	65	80	62	83	119 original
8497	87 [945; beta-D-Glucopyran 126 [559; Erythritol (4TMS)]	43	0.034	0.231	34,840	0.586	78	64	72	70	95	7 original
18236	87 [945; beta-D-Glucopyran 84 Mannitol	60	0.019	0.180	15,946	0.413	79	83	76	68	14	97 duplicate
18179	87 [945; beta-D-Glucopyran 83 Sorbitol	57	-0.004	-0.180	20,047	0.322	80	62	80	52	26	135 duplicate
8511	87 [945; beta-D-Glucopyran 140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	48	-0.005	-0.018	41,160	0.358	81	61	83	59	117	131 original
15931	87 [945; beta-D-Glucopyran 53 Glycerol-2-phosphate	62	-0.014	-0.051	41,483	0.362	82	60	86	58	121	130 duplicate
8480	87 [945; beta-D-Glucopyran 109 Octadecanoic acid	62	-0.046	0.202	21,872	0.409	83	59	73	69	33	88 original
8509	87 [945; beta-D-Glucopyran 138 [674; Ergosterol (1TMS)]	44	-0.049	0.087	40,125	0.386	84	58	81	61	114	108 original
8501	87 [945; beta-D-Glucopyran 130 Trehalose	61	-0.050	-0.052	13,640	0.388	85	57	87	55	10	111 original
16428	87 [945; beta-D-Glucopyran [636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	58	-0.060	-0.153	24,648	0.370	86	56	89	53	41	126 duplicate
8482	87 [945; beta-D-Glucopyran 111 [583; Erythritol (4TMS)]	40	-0.062	-0.006	45,362	0.437	87	55	82	60	132	83 original
10443	87 [945; beta-D-Glucopyran 4 Phosphoric acid	51	-0.062	-0.186	13,806	0.278	88	54	91	51	11	139 duplicate
8464	87 [945; beta-D-Glucopyran 93 [607; Purescine (4TMS)]	58	-0.067	-0.024	45,689	0.406	89	53	84	58	134	99 original
8510	87 [945; beta-D-Glucopyran 139 [700; Ergosta-5,7-dien-3-ol]	37	-0.072	-0.143	40,207	0.386	90	52	88	54	115	113 original
8461	87 [945; beta-D-Glucopyran 90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	62	-0.074	-0.310	32,663	0.433	91	51	96	46	80	84 original
8465	87 [945; beta-D-Glucopyran 94 Hexadecanoic acid	62	-0.087	0.092	19,898	0.401	92	50	79	63	25	103 original
15006	87 [945; beta-D-Glucopyran 43 [548; Leucine (2TBS)]	58	-0.108	-0.217	30,985	0.371	93	49	93	49	73	122 duplicate
8512	87 [945; beta-D-Glucopyran 141 Lanosta-8,24-dien-3-beta-ol	59	-0.115	-0.186	42,946	0.363	94	48	92	50	124	128 original
13318	87 [945; beta-D-Glucopyran 27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	51	-0.191	-0.447	42,498	0.358	95	47	105	37	123	132 duplicate
8508	87 [945; beta-D-Glucopyran 137 Ergosterol	62	-0.193	-0.281	28,626	0.338	96	45	94	48	61	134 original
17687	87 [945; beta-D-Glucopyran 75 Lysine	62	-0.193	-0.282	16,259	0.370	97	46	95	47	15	125 duplicate
13089	87 [945; beta-D-Glucopyran 25 [709; 2,5-Diaminovalerolactam (2TMS)]	46	-0.208	-0.533	40,833	0.577	98	44	115	27	116	10 duplicate
8478	87 [945; beta-D-Glucopyran 107 9-(Z)-Octadecenoic acid	62	-0.214	-0.464	24,801	0.440	99	43	108	34	43	80 original
14299	87 [945; beta-D-Glucopyran 36 [596; N-Acetylglutamic acid (2TMS)]	62	-0.253	-0.361	17,261	0.373	100	42	98	43	17	120 duplicate
8490	87 [945; beta-D-Glucopyran 119 [931; myo-Inositol-2-phosphate (7TMS)]	62	-0.255	-0.431	33,499	0.390	101	41	103	39	88	107 original
8469	87 [945; beta-D-Glucopyran 98 [697; Ribose-5-phosphate methoxamine (5TMS)]	46	-0.256	-0.496	44,157	0.421	102	40	110	32	130	83 original
8495	87 [945; beta-D-Glucopyran 124 [734; 1-Monoleoylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	57	-0.268	-0.359	52,968	0.388	103	39	98	44	140	112 original
8479	87 [945; beta-D-Glucopyran 108 Octadecenoic acid	62	-0.290	-0.449	37,461	0.364	104	38	106	36	108	127 original
15573	87 [945; beta-D-Glucopyran 49 [877; Pyrophosphoric acid (4TMS)]	62	-0.302	-0.522	50,592	0.430	105	37	112	30	138	87 duplicate
10168	87 [945; beta-D-Glucopyran 2 Serine	60	-0.306	-0.391	28,294	0.380	106	36	101	41	60	115 duplicate
17417	87 [945; beta-D-Glucopyran 71 [731; Erythrose (3TMS)]	50	-0.311	-0.339	26,186	0.430	107	35	97	45	53	88 duplicate
16829	87 [945; beta-D-Glucopyran 23 Glutamine	50	-0.322	-0.811	40,102	0.532	108	34	135	7	112	34 duplicate
12856	87 [945; beta-D-Glucopyran 23 Homoserine	62	-0.325	-0.555	34,571	0.439	109	33	118	24	96	81 duplicate
17057	87 [945; beta-D-Glucopyran 66 Glycetic acid-3-phosphate	62	-0.335	-0.418	36,875	0.398	110	32	102	40	105	105 duplicate
15843	87 [945; beta-D-Glucopyran 52 [NA]	44	-0.376	-0.758	43,206	0.490	111	31	130	12	126	53 duplicate
15109	87 [945; beta-D-Glucopyran 45 Homocysteine	59	-0.382	-0.505	51,435	0.353	112	30	111	31	139	133 duplicate
13764	87 [945; beta-D-Glucopyran 31 [622; Parabanic acid (2TMS)]	62	-0.399	-0.546	41,254	0.425	113	29	116	26	118	90 duplicate

8502	87 [945; beta-D-Glucopyran 31	[626; 5-Methylthiadenosine (3TMS)]	53	-0.414	-0.673	45,102	0.522	114	28	125	17	131	38 original
14088	87 [945; beta-D-Glucopyran 34	Aspartic acid	62	-0.419	-0.478	17,486	0.402	115	27	109	33	19	102 duplicate
13873	87 [945; beta-D-Glucopyran 32	[729; N,N-Dimethyllysine methyl ester]	61	-0.423	-0.557	43,470	0.441	116	26	119	23	127	79 duplicate
10981	87 [945; beta-D-Glucopyran 8	Isoleucine	54	-0.434	-0.363	25,535	0.305	117	25	100	42	47	137 duplicate
10848	87 [945; beta-D-Glucopyran 7	Threonine	62	-0.435	-0.445	14,918	0.389	118	24	104	38	12	108 duplicate
11113	87 [945; beta-D-Glucopyran 9	Proline	61	-0.444	-0.463	25,878	0.384	119	23	107	35	51	114 duplicate
12499	87 [945; beta-D-Glucopyran 20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.454	-0.788	32,357	0.370	120	22	133	9	77	123 duplicate
18121	87 [945; beta-D-Glucopyran 82	Lysine	39	-0.466	-0.788	24,663	0.457	121	21	132	10	42	68 duplicate
16592	87 [945; beta-D-Glucopyran 60	Glycerol-3-phosphate	62	-0.475	-0.633	20,087	0.491	122	20	122	20	27	52 duplicate
16511	87 [945; beta-D-Glucopyran 59	Omithine; Arginine	62	-0.488	-0.572	18,030	0.441	123	19	121	21	20	77 duplicate
17278	87 [945; beta-D-Glucopyran 69	Arginine	59	-0.493	-0.856	25,668	0.473	124	18	123	19	50	58 duplicate
13981	87 [945; beta-D-Glucopyran 33	Methionine	62	-0.494	-0.532	34,525	0.406	125	17	114	28	92	100 duplicate
16672	87 [945; beta-D-Glucopyran 61	[NA]	62	-0.520	-0.767	34,539	0.499	126	16	131	11	83	48 duplicate
16104	87 [945; beta-D-Glucopyran 55	[612; 4-Aminobutyric acid (2TBS)]	43	-0.524	-0.888	45,795	0.441	127	15	140	2	135	78 duplicate
8466	87 [945; beta-D-Glucopyran 95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	48	-0.528	-0.728	45,538	0.370	128	14	129	13	133	124 original
15481	87 [945; beta-D-Glucopyran 48	Asparagine	62	-0.535	-0.828	36,980	0.540	129	13	137	5	107	29 duplicate
13654	87 [945; beta-D-Glucopyran 30	[815; Ethyl-3(2H)-thiophenone]	62	-0.542	-0.526	20,870	0.372	130	12	113	29	29	121 duplicate
14908	87 [945; beta-D-Glucopyran 42	Glutamic acid	59	-0.550	-0.558	26,076	0.378	131	11	120	22	52	116 duplicate
8460	87 [945; beta-D-Glucopyran 89	[775; Dopamine (4TMS)]	34	-0.561	-0.877	34,441	0.438	132	10	139	3	80	82 original
18062	87 [945; beta-D-Glucopyran 81	Tyrosine	62	-0.572	-0.794	22,109	0.544	133	9	134	8	34	27 duplicate
17816	87 [945; beta-D-Glucopyran 77	[826; beta-[(5-methyl-2-thienyl)methyl]eneamino-benzeneacetic acid methyl ester]	60	-0.573	-0.877	24,033	0.403	134	8	126	16	39	101 duplicate
10579	87 [945; beta-D-Glucopyran 5	Leucine	45	-0.578	-0.549	32,599	0.274	135	7	117	25	78	140 duplicate
14403	87 [945; beta-D-Glucopyran 37	Phenylalanine	62	-0.583	-0.671	18,478	0.458	136	6	124	18	21	67 duplicate
11244	87 [945; beta-D-Glucopyran 10	Glycine	62	-0.590	-0.823	25,588	0.551	137	5	136	6	48	20 duplicate
17131	87 [945; beta-D-Glucopyran 67	Citric acid	62	-0.616	-0.703	17,415	0.455	138	4	127	15	18	70 duplicate
10306	87 [945; beta-D-Glucopyran 3	Ethanolamine	60	-0.618	-0.830	41,347	0.545	139	3	138	4	120	24 duplicate
15754	87 [945; beta-D-Glucopyran 51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.638	-0.708	43,699	0.401	140	2	128	14	128	104 duplicate
17204	87 [945; beta-D-Glucopyran 68	[570; Hypoxanthine (2TMS)]	20	-0.695	-0.893	27,827	0.363	141	1	141	1	57	129 duplicate
15285	88 Gluconic acid	Arabinose	64	0.778	0.922	7,830	0.680	1	141	5	137	11	8 duplicate
18348	88 Gluconic acid	[793; D-Galactono-1,4-lactone (4TMS)]	61	0.775	0.909	12,818	0.878	2	140	9	133	52	9 duplicate
16983	88 Gluconic acid	[646; 3-Deoxyglucitol (5TMS)]	63	0.774	0.917	11,253	0.681	3	139	8	134	38	7 duplicate
16347	88 Gluconic acid	[757; 2-Desoxy-pentos-3-yose dimethoxyamine (2TMS)]	55	0.768	0.889	8,043	0.659	4	138	14	128	13	18 duplicate
16263	88 Gluconic acid	[829; Orotic acid (3TMS)]	64	0.768	0.923	10,378	0.692	5	137	4	138	30	2 duplicate
8558	88 Gluconic acid	Isomaltose	64	0.765	0.933	15,005	0.688	6	136	1	141	67	5 original
12974	88 Gluconic acid	[725; 2-Ketooctanoic acid (2TMS)]	64	0.763	0.932	23,761	0.706	7	135	2	140	111	1 duplicate
8553	88 Gluconic acid	[840; Maltose methoxyamine (5TMS); alpha-D-Glc-(1,4)-D-Glc]	59	0.755	0.920	8,484	0.664	8	134	7	135	16	16 original
12010	88 Gluconic acid	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	0.753	0.921	9,704	0.691	9	133	6	136	26	3 duplicate
11632	88 Gluconic acid	Uracil	64	0.749	0.928	6,947	0.691	10	132	3	139	5	4 duplicate
15665	88 Gluconic acid	[746; Ribonic acid-1,4-lactone (3TMS)]	50	0.731	0.895	23,016	0.648	11	131	12	130	105	20 duplicate
16019	88 Gluconic acid	[NA]	55	0.714	0.873	14,975	0.606	12	130	17	125	65	44 duplicate
14609	88 Gluconic acid	[828; 1-Phenylethanol (1TMS)]	63	0.701	0.905	6,700	0.636	13	129	10	132	3	26 duplicate
12134	88 Gluconic acid	[700; 2-methyl-1,2-propanediol (2TMS)]	37	0.700	0.880	9,185	0.597	14	128	15	127	22	48 duplicate
16752	88 Gluconic acid	[812; D-Xylofuranose (4TMS)]	62	0.698	0.870	8,353	0.622	15	127	18	124	14	34 duplicate
13544	88 Gluconic acid	Erythritol	64	0.698	0.890	9,653	0.630	16	126	13	129	25	28 duplicate
8523	88 Gluconic acid	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	99	0.673	0.862	14,667	0.634	17	125	20	122	63	28 original
14507	88 Gluconic acid	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.667	0.896	6,395	0.628	18	124	11	131	2	31 duplicate
8527	88 Gluconic acid	[648; Ethylamine (2TMS)]	63	0.659	0.800	8,421	0.573	19	123	27	115	15	66 original



11375	88 Gluconic acid	11 Succinic acid	64 0,658	0,854	7,093	0,571	20	122	23	119	7	67 duplicate
8516	88 Gluconic acid	92 [680; Glyceral-2-phosphate (4TMS)]	54 0,645	0,713	10,330	0,562	21	121	38	104	29	70 original
11504	88 Gluconic acid	12 Glycolic acid	63 0,815	0,861	15,623	0,813	22	120	21	121	71	40 duplicate
11759	88 Gluconic acid	14 Fumaric acid	64 0,606	0,878	13,684	0,613	23	119	16	126	59	41 duplicate
8529	88 Gluconic acid	105 [705; 2-Ketogluconic acid (5TMS)]	68 0,599	0,739	8,856	0,612	24	118	34	108	19	42 original
12739	88 Gluconic acid	22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52 0,585	0,858	15,279	0,618	25	116	22	120	69	37 duplicate
8521	88 Gluconic acid	97 [756; beta-D-Methylglucopyranoside (4TMS)]	52 0,585	0,775	12,348	0,606	26	117	33	109	47	43 original
17880	88 Gluconic acid	78 Mannose	62 0,572	0,775	11,911	0,581	27	115	30	112	42	61 duplicate
17753	88 Gluconic acid	76 Fructose	64 0,559	0,831	16,666	0,643	28	114	24	118	75	23 duplicate
8525	88 Gluconic acid	101 [832; Dopamine (4TMS)]	64 0,555	0,690	8,598	0,539	29	113	42	100	18	76 original
8549	88 Gluconic acid	125 [892; Sucrose (6TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64 0,550	0,767	23,561	0,577	30	112	32	110	110	65 original
8530	88 Gluconic acid	106 [733; Threitol (4TMS)]	62 0,540	0,774	7,179	0,686	32	110	31	111	8	15 original
13432	88 Gluconic acid	28 Malic acid	64 0,539	0,863	6,868	0,622	33	109	19	123	4	35 duplicate
8539	88 Gluconic acid	115 Glucose-6-phosphate	62 0,530	0,798	16,791	0,628	34	108	28	114	76	30 original
17555	88 Gluconic acid	73 [708; Glucose methoxamine (5TMS)]	57 0,526	0,887	10,518	0,528	35	107	45	97	32	81 duplicate
14195	88 Gluconic acid	35 Pyroglutamic acid	64 0,519	0,806	33,974	0,634	36	106	28	116	138	27 duplicate
14710	88 Gluconic acid	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	64 0,515	0,782	27,894	0,599	37	105	29	113	128	47 duplicate
8515	88 Gluconic acid	91 [766; beta-D-Methylglucopyranoside (4TMS)]	64 0,513	0,685	12,709	0,511	38	104	46	98	51	92 original
17348	88 Gluconic acid	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57 0,509	0,545	12,999	0,489	39	103	59	83	55	103 duplicate
10030	88 Gluconic acid	1 [938; Sulfuric acid (2TMS)]	36 0,495	0,828	12,402	0,594	40	102	53	89	48	51 duplicate
8552	88 Gluconic acid	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45 0,493	0,689	7,482	0,593	41	101	43	99	9	52 original
8544	88 Gluconic acid	120 [945; Uridine (3TMS)]	54 0,488	0,732	8,541	0,591	42	100	72	70	17	55 original
12620	88 Gluconic acid	21 [878; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64 0,480	0,732	10,536	0,554	43	99	35	107	33	73 duplicate
13205	88 Gluconic acid	26 Citramalic acid	64 0,465	0,727	11,433	0,517	44	98	36	106	39	89 duplicate
18402	88 Gluconic acid	87 [945; beta-D-Glucopyranose (5TMS)]	62 0,461	0,720	27,372	0,500	45	97	37	105	124	100 duplicate
8534	88 Gluconic acid	110 [715; Erythritol (4TMS)]	54 0,430	0,682	22,046	0,528	46	96	40	102	60	6 original
8536	88 Gluconic acid	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63 0,430	0,682	22,046	0,528	47	95	47	95	101	82 original
8528	88 Gluconic acid	102 [904; Galactose methoxamine (5TMS)]	64 0,423	0,610	11,849	0,537	48	94	55	87	41	77 original
8541	88 Gluconic acid	117 [724; Glycerol (3TMS)]	56 0,417	0,662	11,031	0,581	49	93	50	92	38	59 original
10715	88 Gluconic acid	6 Glycerol	64 0,415	0,667	34,760	0,522	50	92	49	93	140	87 duplicate
8524	88 Gluconic acid	100 [857; Mannitol (6TMS)]	64 0,413	0,688	7,607	0,554	51	91	44	98	10	72 original
8548	88 Gluconic acid	122 [844; Erythritol (4TMS)]	52 0,412	0,708	19,592	0,605	52	90	39	103	92	45 original
18283	88 Gluconic acid	85 [529; Methyldiacetic acid (4TMS)]	48 0,394	0,661	5,828	0,526	53	89	51	91	1	83 duplicate
8545	88 Gluconic acid	121 [657; Erythritol (4TMS)]	55 0,386	0,610	18,756	0,581	54	88	56	86	85	60 original
15104	88 Gluconic acid	44 [910; 2-Ketogluconic acid methoxamine (4TMS)]	50 0,373	0,618	9,490	0,614	55	87	54	88	24	38 duplicate
8556	88 Gluconic acid	132 [895; Isomaltose methoxamine (8TMS)]	42 0,370	0,828	18,518	0,577	56	86	25	117	83	64 original
8537	88 Gluconic acid	113 Galactose-6-phosphate	62 0,358	0,678	11,953	0,584	57	85	48	94	43	57 original
8551	88 Gluconic acid	127 [777; Fructose-6-phosphate methoxamine (6TMS)]	39 0,333	0,501	10,437	0,596	58	84	65	77	31	49 original
12257	88 Gluconic acid	18 [590; 1-Acetyl-2-thiohydantoin]	64 0,331	0,502	8,732	0,428	59	83	64	78	20	128 duplicate
8559	88 Gluconic acid	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64 0,322	0,514	9,457	0,507	60	82	63	79	23	94 original
12378	88 Gluconic acid	19 Alanine (BP) (3TMS)	64 0,319	0,585	8,010	0,579	61	81	57	85	12	62 duplicate
8540	88 Gluconic acid	116 [882; Pseudouridine (5TMS)]	30 0,287	0,349	9,960	0,459	62	80	71	71	28	115 original
8528	88 Gluconic acid	104 [795; Erythritol (4TMS)]	63 0,276	0,381	10,635	0,568	63	79	70	72	34	68 original
18003	88 Gluconic acid	80 [772; D-Glucose (5TMS)]	62 0,267	0,583	23,261	0,462	64	78	58	84	107	114 duplicate
8538	88 Gluconic acid	114 Fructose-6-phosphate	53 0,266	0,644	13,108	0,592	65	77	52	90	56	54 original
17622	88 Gluconic acid	74 [912; Tetradecanoic acid (1TMS)]	64 0,261	0,532	12,224	0,544	66	76	60	82	44	75 duplicate
14810	88 Gluconic acid	41 [839; Proline (2TMS)]	64 0,235	0,422	9,756	0,506	67	75	66	76	27	95 duplicate
8547	88 Gluconic acid	123 [945; Galactofuranose-6-phosphate (7TMS)]	64 0,212	0,415	8,802	0,593	68	74	67	75	21	53 original
15389	88 Gluconic acid	47 [NA]	64 0,200	0,271	12,944	0,495	69	73	76	66	54	101 duplicate
8520	88 Gluconic acid	96 myo-inositol	49 0,194	0,222	23,125	0,312	70	72	78	84	108	141 original

8517	88	Gluconic acid	93	[607: Putrescine (4TMS)]	60	0.180	0.384	21.372	0.466	71	71	69	73	98	112 original
18180	88	Gluconic acid	83	Sorbitol	58	0.175	-0.358	18.974	0.401	72	70	93	49	87	131 duplicate
8550	88	Gluconic acid	126	[559: Erythritol (4TMS)]	45	0.174	0.401	13.518	0.653	73	69	68	74	58	19 original
18237	88	Gluconic acid	84	Mannitol	62	0.157	0.524	24.510	0.525	74	68	61	81	115	85 duplicate
8535	88	Gluconic acid	111	[583: Erythritol (4TMS)]	42	0.145	0.276	25.468	0.375	75	67	75	67	122	138 original
11865	88	Gluconic acid	15	Alanine	64	0.134	0.312	13.473	0.638	76	66	73	69	57	25 duplicate
17842	88	Gluconic acid	79	Glucose	64	0.111	0.517	27.789	0.642	77	65	62	80	127	24 duplicate
16907	88	Gluconic acid	64	[789: Tyramine (3TMS)]	63	0.108	0.227	11.688	0.434	78	64	77	65	40	125 duplicate
8557	88	Gluconic acid	133	[855: Squalene]	64	0.054	0.002	12.275	0.401	79	63	86	56	48	132 original
8533	88	Gluconic acid	109	Octadecanoic acid	64	0.052	0.291	17.422	0.525	80	62	74	68	79	84 original
8564	88	Gluconic acid	140	[692: Ergosta-7,22-dien-3-ol (1TMS)]	49	0.037	0.170	19.948	0.483	81	61	80	82	94	107 original
8514	88	Gluconic acid	90	[910: 9-(Z)-Hexadecenoic acid (1TMS)]	64	0.036	0.047	10.937	0.416	82	60	82	60	35	130 original
15932	88	Gluconic acid	53	Glycerol-2-phosphate	64	0.028	0.016	17.209	0.400	83	59	85	57	78	133 duplicate
8518	88	Gluconic acid	94	Hexadecanoic acid	64	-0.019	0.210	16.612	0.523	84	58	79	63	73	88 original
8542	88	Gluconic acid	118	[928: Glucopyranose-6-phosphate (6TMS)]	58	-0.039	0.140	14.555	0.457	85	57	81	61	62	118 original
8565	88	Gluconic acid	141	Lanosta-8,24-dien-3-beta-ol	61	-0.055	0.017	19.493	0.513	86	56	84	58	91	91 original
8582	88	Gluconic acid	138	[674: Ergosterol (1TMS)]	46	-0.067	0.040	21.305	0.436	87	55	83	59	97	122 original
17487	88	Gluconic acid	72	[919: D-Xylopyranose (4TMS)]	63	-0.081	-0.158	15.575	0.393	88	54	91	51	70	135 duplicate
8531	88	Gluconic acid	107	9-(Z)-Octadecenoic acid	64	-0.085	-0.191	12.230	0.393	89	53	92	50	45	134 original
8563	88	Gluconic acid	139	[700: Ergosta-5,7-dien-3-ol]	38	-0.087	-0.114	22.852	0.431	90	52	89	53	104	127 original
8543	88	Gluconic acid	119	[931: myo-Inositol-2-phosphate (7TMS)]	64	-0.091	-0.086	12.412	0.520	91	51	88	54	49	88 original
16830	88	Gluconic acid	63	Glutamine	52	-0.095	-0.681	24.055	0.647	92	50	118	24	112	21 duplicate
8561	88	Gluconic acid	137	Ergosterol	64	-0.112	-0.064	13.987	0.454	93	49	87	55	61	119 original
15844	88	Gluconic acid	52	[NA]	46	-0.188	-0.569	26.308	0.667	94	48	104	38	123	14 duplicate
8548	88	Gluconic acid	124	[734: 1-Monooctylethanol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	59	-0.207	-0.358	29.376	0.416	95	47	94	48	133	129 original
15007	88	Gluconic acid	43	[548: Leucine (2TBS)]	60	-0.208	-0.375	12.447	0.487	96	46	96	46	50	104 duplicate
17418	88	Gluconic acid	71	[731: Erythrose (3TMS)]	64	-0.225	-0.379	11.057	0.507	97	45	97	45	37	93 duplicate
10444	88	Gluconic acid	4	Phosphoric acid	51	-0.231	-0.493	29.682	0.389	98	44	101	41	134	140 duplicate
8560	88	Gluconic acid	136	[748: D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.235	-0.117	6.952	0.431	99	43	90	52	6	128 original
8554	88	Gluconic acid	130	Trehalose	63	-0.252	-0.373	24.324	0.393	100	42	95	47	113	136 original
16430	88	Gluconic acid	58	[636: 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	-0.291	-0.473	15.849	0.437	101	41	100	42	72	121 duplicate
13319	88	Gluconic acid	27	[815: (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	-0.295	-0.728	24.989	0.564	102	40	121	21	119	69 duplicate
8532	88	Gluconic acid	108	Octadecenoic acid	64	-0.301	-0.429	15.169	0.384	103	39	88	44	68	137 original
13090	88	Gluconic acid	25	[709: 2,5-Diaminovalerolactam (2TMS)]	48	-0.307	-0.812	23.473	0.625	104	38	129	13	109	32 duplicate
16673	88	Gluconic acid	61	[NA]	64	-0.323	-0.460	12.830	0.474	105	37	99	43	53	110 duplicate
8522	88	Gluconic acid	88	[697: Ribose-5-phosphate methoxamine (5TMS)]	48	-0.328	-0.733	24.884	0.559	106	36	122	20	117	71 original
14300	88	Gluconic acid	36	[596: N-Acetylglutamic acid (2TMS)]	64	-0.344	-0.627	24.933	0.470	107	35	111	31	118	111 duplicate
15574	88	Gluconic acid	49	[877: Pyrophosphoric acid (4TMS)]	64	-0.346	-0.510	27.642	0.504	108	34	102	40	126	97 duplicate
17688	88	Gluconic acid	75	Lysine	64	-0.353	-0.577	34.450	0.492	109	33	106	38	139	102 duplicate
10849	88	Gluconic acid	7	Threonine	64	-0.390	-0.578	25.124	0.436	110	32	107	35	121	123 duplicate
12857	88	Gluconic acid	23	Homoserine	64	-0.398	-0.790	18.093	0.578	111	31	128	16	82	63 duplicate
8513	88	Gluconic acid	89	[775: Dopamine (4TMS)]	35	-0.405	-0.821	21.738	0.587	112	30	131	11	99	56 original
10169	88	Gluconic acid	2	Serine	62	-0.408	-0.653	21.755	0.457	113	29	113	29	100	117 duplicate
17058	88	Gluconic acid	66	Glyceric acid-3-phosphate	64	-0.411	-0.674	14.789	0.483	114	28	116	26	64	106 duplicate
15200	88	Gluconic acid	45	Homocysteine	61	-0.414	-0.574	27.828	0.440	115	27	105	37	128	120 duplicate
17205	88	Gluconic acid	68	[570: Hypoxanthine (2TMS)]	20	-0.421	-0.917	17.203	0.644	116	26	140	2	77	22 duplicate
10982	88	Gluconic acid	8	Isoleucine	55	-0.433	-0.523	19.949	0.371	117	25	103	39	95	139 duplicate
8519	88	Gluconic acid	95	[770: 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	-0.447	-0.652	24.742	0.582	118	24	112	30	116	58 original
13765	88	Gluconic acid	31	[622: Parabenic acid (2TMS)]	64	-0.460	-0.712	18.925	0.483	119	23	120	22	86	105 duplicate

17132	88 Gluconic acid	67 Citric acid	64 -0.464	-0.670	19,196	0.465	120	22	115	27	88	113 duplicate
18693	88 Gluconic acid	60 Glycero-3-phosphate	64 -0.466	-0.611	18,069	0.536	121	21	109	33	81	78 duplicate
14089	88 Gluconic acid	34 Aspartic acid	64 -0.481	-0.610	28,721	0.476	122	20	108	34	131	109 duplicate
8555	88 Gluconic acid	131 [626; 5-Methylthioadenosine (3TMS)]	55 -0.490	-0.623	22,500	0.622	123	19	110	32	102	36 original
15482	88 Gluconic acid	48 Asparagine	64 -0.490	-0.785	19,482	0.662	124	18	127	15	90	17 duplicate
14404	88 Gluconic acid	37 Phenylalanine	64 -0.491	-0.678	18,688	0.516	125	17	117	25	84	80 duplicate
13982	88 Gluconic acid	33 Methionine	64 -0.534	-0.669	17,703	0.504	126	16	114	28	80	98 duplicate
11114	88 Gluconic acid	9 Proline	63 -0.561	-0.758	28,042	0.481	127	15	124	18	130	108 duplicate
15755	88 Gluconic acid	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44 -0.575	-0.850	23,340	0.550	128	14	136	6	108	74 duplicate
13655	88 Gluconic acid	30 [815; Ethyl-3(2H)-thiophenone]	64 -0.581	-0.695	27,569	0.458	129	13	119	23	125	116 duplicate
13874	88 Gluconic acid	32 [729; N,N-Dimethyllysine methyl ester]	63 -0.582	-0.816	25,047	0.604	130	12	130	12	120	46 duplicate
17277	88 Gluconic acid	69 Arginine	60 -0.611	-0.850	22,500	0.624	131	11	135	7	103	33 duplicate
10580	88 Gluconic acid	5 Leucine	45 -0.616	-0.806	14,996	0.534	132	10	128	14	66	79 duplicate
10307	88 Gluconic acid	3 Ethanolamine	62 -0.622	-0.828	19,779	0.596	133	9	133	9	93	50 duplicate
16512	88 Gluconic acid	59 Ornithine; Arginine	64 -0.633	-0.744	35,962	0.503	134	8	123	19	141	99 duplicate
16105	88 Gluconic acid	55 [612; 4-Aminobutyric acid (2TBS)]	43 -0.650	-0.839	24,340	0.617	135	7	134	8	114	38 duplicate
11245	88 Gluconic acid	10 Glycine	64 -0.653	-0.905	19,432	0.668	136	6	136	4	89	13 duplicate
17817	88 Gluconic acid	77 benzeneacetic acid methyl ester	62 -0.658	-0.824	29,074	0.505	137	5	132	10	132	96 duplicate
12500	88 Gluconic acid	20 [619; 2-{3',4'-Bishydroxyphenyl}-2-oxoethylamine (4TMS)]	31 -0.660	-0.910	16,648	0.678	138	4	139	3	74	10 duplicate
18063	88 Gluconic acid	81 Tyrosine	64 -0.664	-0.865	31,523	0.669	139	3	137	5	137	12 duplicate
14909	88 Gluconic acid	42 Glutamic acid	60 -0.707	-0.775	30,014	0.531	140	2	125	17	136	80 duplicate
18122	88 Gluconic acid	82 Lysine	39 -0.735	-0.963	19,965	0.676	141	1	141	1	96	11 duplicate
8571	89 [775; Dopamine (4TMS)]	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	26 -0.846	0.881	10,368	0.616	1	140	9	132	10	12 original
16831	89 [775; Dopamine (4TMS)]	63 Glutamine	31 -0.759	0.984	6,343	0.566	2	139	1	140	2	37 duplicate
10081	89 [775; Dopamine (4TMS)]	5 Leucine	29 -0.749	0.740	9,829	0.520	3	138	14	127	8	58 duplicate
15845	89 [775; Dopamine (4TMS)]	52 [NA]	27 -0.721	0.980	5,198	0.647	4	137	3	138	1	6 duplicate
16106	89 [775; Dopamine (4TMS)]	55 [612; 4-Aminobutyric acid (2TBS)]	26 -0.686	0.967	9,768	0.651	5	136	4	137	7	5 duplicate
15463	89 [775; Dopamine (4TMS)]	48 Asparagine	35 -0.661	0.894	12,539	0.602	6	135	7	134	18	18 duplicate
11248	89 [775; Dopamine (4TMS)]	10 Glycine	35 -0.630	0.886	21,464	0.605	7	134	8	133	84	17 duplicate
15575	89 [775; Dopamine (4TMS)]	49 [877; Pyrophosphoric acid (4TMS)]	35 -0.624	0.739	9,589	0.451	8	133	15	126	6	84 duplicate
18123	89 [775; Dopamine (4TMS)]	82 Lysine	28 -0.619	0.944	15,436	0.664	9	132	6	135	39	2 duplicate
15201	89 [775; Dopamine (4TMS)]	45 Homocysteine	34 -0.608	0.634	13,712	0.427	10	131	23	118	26	107 duplicate
17206	89 [775; Dopamine (4TMS)]	81 Tyrosine	15 -0.581	0.983	12,342	0.586	11	130	2	139	16	25 duplicate
18084	89 [775; Dopamine (4TMS)]	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	35 -0.573	0.770	34,108	0.670	12	129	12	129	134	1 duplicate
15756	89 [775; Dopamine (4TMS)]	30 [815; Ethyl-3(2H)-thiophenone]	29 -0.571	0.728	12,596	0.524	13	128	16	125	19	56 duplicate
13656	89 [775; Dopamine (4TMS)]	61 [NA]	35 -0.570	0.625	31,497	0.543	14	127	25	116	128	45 duplicate
16674	89 [775; Dopamine (4TMS)]	3 Ethanolamine	35 -0.566	0.756	14,465	0.503	15	126	13	128	30	70 duplicate
10308	89 [775; Dopamine (4TMS)]	33 Methionine	34 -0.533	0.857	10,330	0.659	16	125	10	131	9	4 duplicate
13983	89 [775; Dopamine (4TMS)]	77 benzeneacetic acid methyl ester	35 -0.519	0.623	16,115	0.544	17	124	26	115	47	44 duplicate
17818	89 [775; Dopamine (4TMS)]	131 [626; 5-Methylthioadenosine (3TMS)]	34 -0.519	0.683	31,170	0.566	18	123	20	121	125	36 duplicate
8607	89 [775; Dopamine (4TMS)]	69 Arginine	28 -0.497	0.850	9,396	0.622	19	122	11	130	5	10 original
17278	89 [775; Dopamine (4TMS)]	25 [709; 2,5-Diaminovalerolactam (2TMS)]	35 -0.492	0.717	23,271	0.571	20	121	17	124	99	34 duplicate
13091	89 [775; Dopamine (4TMS)]	23 Homoserine	19 -0.485	0.651	9,260	0.404	21	120	22	119	4	115 duplicate
12858	89 [775; Dopamine (4TMS)]	34 Aspartic acid	35 -0.476	0.687	13,527	0.534	22	118	19	122	24	52 duplicate
14090	89 [775; Dopamine (4TMS)]	98 [697; Ribose-5-phosphate methoxamine (5TMS)]	35 -0.476	0.589	33,402	0.537	23	119	29	112	131	49 duplicate
8574	89 [775; Dopamine (4TMS)]	8 Isoleucine	26 -0.458	0.634	11,507	0.498	24	117	24	117	11	72 original
10983	89 [775; Dopamine (4TMS)]	42 Glutamic acid	34 -0.451	0.288	21,788	0.459	25	116	44	97	88	87 duplicate
14910	89 [775; Dopamine (4TMS)]		35 -0.448	0.561	30,680	0.530	26	115	31	110	123	54 duplicate

8569	89 [775; Dopamine (4TMS) 93	[607; Putrescine (4TMS)]	32	0.448	0.221	13.301	0.514	27	114	47	94	22'	61 original
11115	89 [775; Dopamine (4TMS) 9	Proline	34	0.437	0.401	28.958	0.579	28	113	39	102	115	31 duplicate
13766	89 [775; Dopamine (4TMS) 31	[622; Parabanic acid (2TMS)]	35	0.435	0.523	12.420	0.412	29	112	35	106	17	112 duplicate
13875	89 [775; Dopamine (4TMS) 32	[729; N,N-Dimethyllysine methyl ester]	35	0.429	0.592	12.098	0.582	30	111	28	113	14	28 duplicate
16513	89 [775; Dopamine (4TMS) 59	Ornithine; Arginine	35	0.402	0.655	39.002	0.549	31	110	21	120	140	42 duplicate
17133	89 [775; Dopamine (4TMS) 67	Citric acid	35	0.398	0.594	26.828	0.549	32	109	27	114	113	41 duplicate
8561	89 [775; Dopamine (4TMS) 105	[705; 2-Ketogluconic acid (5TMS)]	19	0.380	0.713	17.746	0.511	33	108	18	123	58	62 original
14405	89 [775; Dopamine (4TMS) 37	Phenylalanine	35	0.375	0.465	26.287	0.508	34	107	38	103	111	68 duplicate
12501	89 [775; Dopamine (4TMS) 20	[618; 2,3',4'-Bishydroxyphenyl]-2-oxoethylamine (4TMS)]	23	0.344	0.965	7.498	0.664	35	106	5	136	3	3 duplicate
17059	89 [775; Dopamine (4TMS) 66	Glyceric acid-3-phosphate	35	0.334	0.353	14.131	0.438	36	105	42	99	28	100 duplicate
13320	89 [775; Dopamine (4TMS) 27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	34	0.305	0.587	11.635	0.443	37	104	30	111	12	99 duplicate
15933	89 [775; Dopamine (4TMS) 53	Glycerol-2-phosphate	35	0.304	0.487	12.603	0.341	38	103	38	105	20	132 duplicate
8584	89 [775; Dopamine (4TMS) 108	Octadecenoic acid	35	0.291	0.532	13.401	0.388	39	102	34	107	23	121 original
10170	89 [775; Dopamine (4TMS) 2	Serine	35	0.284	0.241	22.307	0.510	40	101	46	95	96	64 duplicate
8595	89 [775; Dopamine (4TMS) 119	[931; myo-Inositol-2-phosphate (7TMS)]	35	0.267	0.536	15.992	0.452	41	100	32	109	46	93 original
8566	89 [775; Dopamine (4TMS) 90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	35	0.250	0.482	15.455	0.428	42	99	37	104	40	106 original
8583	89 [775; Dopamine (4TMS) 107	9-(Z)-Octadecenoic acid	35	0.247	0.535	20.452	0.336	43	98	33	108	79	134 original
15008	89 [775; Dopamine (4TMS) 43	[548; Leucine (2TMS)]	34	0.244	0.367	15.146	0.540	44	97	41	100	35	46 duplicate
10031	89 [775; Dopamine (4TMS) 1	[938; Sulfuric acid (2TMS)]	16	0.217	-0.290	12.156	0.367	45	96	68	73	15	122 duplicate
16594	89 [775; Dopamine (4TMS) 60	Glycerol-3-phosphate	35	0.193	0.380	25.705	0.498	46	95	40	101	110	73 duplicate
18238	89 [775; Dopamine (4TMS) 84	Mannitol	34	0.184	0.086	29.529	0.461	47	94	55	86	117	84 duplicate
8604	89 [775; Dopamine (4TMS) 128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	19	0.135	-0.398	17.838	0.390	48	93	71	70	60	120 original
10850	89 [775; Dopamine (4TMS) 7	Threonine	35	0.106	0.131	31.496	0.518	49	92	60	91	127	59 duplicate
8603	89 [775; Dopamine (4TMS) 127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	18	0.046	0.110	14.478	0.353	50	91	52	89	31	129 original
8573	89 [775; Dopamine (4TMS) 97	[756; beta-D-Methylglucopyranoside (4TMS)]	23	0.036	-0.588	25.199	0.532	51	90	80	61	108	53 original
14301	89 [775; Dopamine (4TMS) 36	[596; N-Acetylglutamic acid (2TMS)]	35	0.015	0.248	29.827	0.463	52	89	45	96	119	83 duplicate
8606	89 [775; Dopamine (4TMS) 130	Trehalose	34	-0.005	0.167	30.453	0.346	53	88	48	93	122	130 original
17488	89 [775; Dopamine (4TMS) 72	[919; D-Xylopyranose (4TMS)]	35	-0.008	0.155	14.601	0.277	54	87	49	92	33	140 duplicate
8600	89 [775; Dopamine (4TMS) 124	[734; 1-Monocoleoylglycerol (2TMS); 1-Monohexadecenoylethanol (1TMS)]	35	-0.015	0.313	15.849	0.371	55	86	43	98	43	126 original
15390	89 [775; Dopamine (4TMS) 47	[NA]	35	-0.018	-0.015	16.775	0.420	56	85	58	83	54	109 duplicate
8575	89 [775; Dopamine (4TMS) 99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	21	-0.076	-0.622	14.333	0.369	57	84	85	56	29	127 original
17419	89 [775; Dopamine (4TMS) 71	[731; Erythrose (3TMS)]	35	-0.079	-0.099	19.816	0.478	58	83	61	80	75	77 duplicate
10445	89 [775; Dopamine (4TMS) 4	Phosphoric acid	31	-0.110	0.099	33.429	0.372	59	82	54	87	132	125 duplicate
17689	89 [775; Dopamine (4TMS) 75	Lysine	35	-0.123	0.036	37.932	0.461	60	81	56	85	137	85 duplicate
8613	89 [775; Dopamine (4TMS) 137	Ergosterol	35	-0.126	0.123	20.899	0.383	61	80	51	90	82	123 original
8612	89 [775; Dopamine (4TMS) 136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	13	-0.128	-0.222	13.133	0.285	62	79	65	76	21	139 original
8615	89 [775; Dopamine (4TMS) 139	[700; Ergosta-5,7-dien-3-ol]	24	-0.167	-0.017	13.683	0.344	63	78	59	82	25	131 original
8617	89 [775; Dopamine (4TMS) 141	Lanosta-8,24-dien-3-beta-ol	34	-0.184	0.104	13.977	0.415	64	77	53	88	27	111 original
8596	89 [775; Dopamine (4TMS) 126	[845; Uridine (3TMS)]	27	-0.185	-0.120	18.926	0.328	65	76	62	79	69	135 original
8602	89 [775; Dopamine (4TMS) 120	[559; Erythritol (4TMS)]	19	-0.205	-0.304	15.270	0.455	66	75	69	72	37	91 original
8568	89 [775; Dopamine (4TMS) 92	[680; Glycerol-2-phosphate (4TMS)]	25	-0.213	-0.906	19.466	0.509	67	74	130	11	73	68 original
8577	89 [775; Dopamine (4TMS) 101	[832; Dopamine (4TMS)]	35	-0.261	-0.532	19.313	0.588	68	72	77	64	72	23 original
13545	89 [775; Dopamine (4TMS) 29	Erythritol	35	-0.261	-0.707	16.350	0.454	69	73	94	47	50	92 duplicate
8570	89 [775; Dopamine (4TMS) 94	Hexadecenoic acid	35	-0.264	-0.452	28.037	0.501	70	71	72	69	114	71 original
8579	89 [775; Dopamine (4TMS) 103	[648; Ethylamine (2TMS)]	34	-0.269	-0.640	22.259	0.571	71	70	87	54	95	33 original
16431	89 [775; Dopamine (4TMS) 58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	35	-0.271	-0.221	22.016	0.470	72	69	64	77	90	80 duplicate
16348	89 [775; Dopamine (4TMS) 57	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	26	-0.274	-0.843	23.588	0.445	73	68	115	26	101	88 duplicate

[illegible]

13433	89 [775; Dopamine (4TMS)]	28	Malic acid	35	-0.553	-0.804	19,058	0.581	123	18	108	33	70	30 duplicate
18403	89 [775; Dopamine (4TMS)]	87	[945; beta-D-Glucopyranose (5TMS)]	34	-0.561	-0.877	34,441	0.438	124	17	123	18	136	101 duplicate
10716	89 [775; Dopamine (4TMS)]	6	Glycerol	35	-0.563	-0.901	38,754	0.482	125	15	129	12	138	76 duplicate
8601	89 [775; Dopamine (4TMS)]	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	35	-0.563	-0.972	33,127	0.561	126	16	140	1	130	38 original
8597	89 [775; Dopamine (4TMS)]	121	[657; Erythritol (4TMS)]	28	-0.577	-0.787	16,567	0.506	127	14	103	38	53	69 original
17943	89 [775; Dopamine (4TMS)]	79	Glucose	35	-0.583	-0.940	34,377	0.557	128	13	135	6	135	39 duplicate
18004	89 [775; Dopamine (4TMS)]	80	[772; D-Glucose (5TMS)]	34	-0.597	-0.848	31,480	0.417	129	12	116	25	126	110 duplicate
8589	89 [775; Dopamine (4TMS)]	113	Galactose-6-phosphate	34	-0.608	-0.945	20,099	0.582	130	11	138	3	77	29 original
17881	89 [775; Dopamine (4TMS)]	78	Mannose	34	-0.611	-0.898	21,148	0.544	131	10	128	13	83	43 duplicate
8593	89 [775; Dopamine (4TMS)]	117	[724; Glyceral (3TMS)]	28	-0.614	-0.814	18,670	0.488	132	9	111	30	68	74 original
8590	89 [775; Dopamine (4TMS)]	114	Fructose-6-phosphate	30	-0.623	-0.923	18,583	0.568	133	8	134	7	66	35 original
17349	89 [775; Dopamine (4TMS)]	70	[893; 2-Furan-2-hydroxyacetic acid (2TMS)]	32	-0.633	-0.911	23,524	0.437	134	7	131	10	100	102 duplicate
14811	89 [775; Dopamine (4TMS)]	41	[639; Proline (2TMS)]	35	-0.637	-0.747	22,395	0.450	135	5	97	44	97	95 duplicate
17754	89 [775; Dopamine (4TMS)]	76	Fructose	35	-0.637	-0.956	30,350	0.583	136	6	139	2	121	27 duplicate
8582	89 [775; Dopamine (4TMS)]	106	[733; Threitol (4TMS)]	35	-0.671	-0.883	22,196	0.625	137	4	125	16	92	9 original
8580	89 [775; Dopamine (4TMS)]	104	[795; Erythritol (4TMS)]	35	-0.681	-0.856	18,561	0.596	138	3	118	23	65	19 original
8599	89 [775; Dopamine (4TMS)]	123	[945; Galactofuranose-6-phosphate (7TMS)]	35	-0.684	-0.913	20,450	0.630	139	2	132	9	78	7 original
12380	89 [775; Dopamine (4TMS)]	19	Alanine (BP) (3TMS)	35	-0.724	-0.877	22,235	0.508	140	1	124	17	84	67 duplicate
8634	90 [910; 9-(Z)-Hexadecano	107	9-(Z)-Octadecanoic acid	64	0.738	0.885	9,503	0.587	1	141	1	141	27	1 original
12502	90 [910; 9-(Z)-Hexadecano	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	0.544	0.552	14,531	0.549	2	140	5	137	70	2 duplicate
8646	90 [910; 9-(Z)-Hexadecano	119	[931; myo-Inositol-2-phosphate (7TMS)]	64	0.498	0.683	4,446	0.514	3	139	2	140	3	3 original
8635	90 [910; 9-(Z)-Hexadecano	108	Octadecanoic acid	64	0.368	0.504	6,888	0.394	4	138	7	135	13	59 original
18239	90 [910; 9-(Z)-Hexadecano	84	Mannitol	62	0.355	0.352	27,676	0.355	5	137	20	122	128	100 duplicate
18832	90 [910; 9-(Z)-Hexadecano	63	Glutamine	52	0.353	0.478	14,706	0.418	6	136	11	131	72	41 duplicate
8655	90 [910; 9-(Z)-Hexadecano	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.337	0.267	7,431	0.360	7	135	28	114	17	98 original
15846	90 [910; 9-(Z)-Hexadecano	52	[NA]	46	0.335	0.554	19,090	0.450	8	134	4	138	100	13 duplicate
8632	90 [910; 9-(Z)-Hexadecano	105	[705; 2-Ketogluconic acid (5TMS)]	48	0.333	0.469	10,534	0.377	9	133	12	130	36	76 original
8684	90 [910; 9-(Z)-Hexadecano	137	Ergosterol	64	0.326	0.499	10,263	0.422	10	132	8	134	33	37 original
8620	90 [910; 9-(Z)-Hexadecano	93	[607; Putrescine (4TMS)]	60	0.319	0.315	16,759	0.354	11	131	24	118	88	102 original
8621	90 [910; 9-(Z)-Hexadecano	94	Hexadecanoic acid	64	0.305	0.189	17,982	0.514	12	130	33	109	96	4 original
8651	90 [910; 9-(Z)-Hexadecano	124	[734; 1-Monoleoylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	59	0.305	0.423	24,243	0.417	13	129	13	129	119	43 original
8626	90 [910; 9-(Z)-Hexadecano	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	0.293	0.392	10,525	0.372	14	128	16	126	35	83 original
8654	90 [910; 9-(Z)-Hexadecano	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.277	0.397	4,750	0.341	15	127	15	127	4	117 original
8659	90 [910; 9-(Z)-Hexadecano	132	[895; Isomaltose methoxyamine (6TMS)]	42	0.273	0.365	15,149	0.366	16	126	19	123	76	66 original
18124	90 [910; 9-(Z)-Hexadecano	82	Lysine	39	0.269	0.407	13,678	0.495	17	125	14	128	64	6 duplicate
8668	90 [910; 9-(Z)-Hexadecano	141	Lanosta-8,24-dien-3-beta-ol	61	0.268	0.506	14,108	0.402	18	124	6	136	68	54 original
15934	90 [910; 9-(Z)-Hexadecano	53	Glycerol-2-phosphate	64	0.254	0.314	11,285	0.393	19	123	25	117	49	62 duplicate
8636	90 [910; 9-(Z)-Hexadecano	109	Octadecanoic acid	64	0.252	0.057	19,691	0.502	20	122	57	85	106	5 original
18509	90 [910; 9-(Z)-Hexadecano	89	[775; Dopamine (4TMS)]	35	0.250	0.482	15,455	0.428	21	121	10	132	77	31 duplicate
8638	90 [910; 9-(Z)-Hexadecano	111	[583; Erythritol (4TMS)]	42	0.245	0.376	19,300	0.425	22	120	18	124	102	33 original
8653	90 [910; 9-(Z)-Hexadecano	126	[559; Erythritol (4TMS)]	45	0.236	0.284	7,845	0.365	23	119	27	115	18	67 original
10032	90 [910; 9-(Z)-Hexadecano	1	[938; Sulfuric acid (2TMS)]	36	0.232	0.338	7,897	0.355	24	118	21	121	19	101 duplicate
16021	90 [910; 9-(Z)-Hexadecano	54	[NA]	55	0.224	0.117	12,974	0.418	25	117	43	99	60	42 duplicate
16349	90 [910; 9-(Z)-Hexadecano	57	[757; 2-Deoxy-pentose-3-ylose dimethoxyamine (2TMS)]	55	0.223	0.158	13,890	0.407	26	116	38	104	67	48 duplicate
16107	90 [910; 9-(Z)-Hexadecano	55	[612; 4-Aminobutyric acid (2TBS)]	43	0.209	0.557	21,099	0.470	27	115	3	139	113	8 duplicate
8658	90 [910; 9-(Z)-Hexadecano	131	[626; 5-Methylthioadenosine (3TMS)]	55	0.196	0.324	16,268	0.403	28	114	22	120	84	52 original
10582	90 [910; 9-(Z)-Hexadecano	5	Leucine	45	0.194	0.098	10,257	0.341	29	113	47	95	32	119 duplicate
16675	90 [910; 9-(Z)-Hexadecano	61	[NA]	64	0.177	0.213	5,286	0.364	30	112	31	111	5	89 duplicate

8643	90 [910; 9-(Z)-Hexadeceno	116 [862; Pseudouridine (5TMS)]	30	0.172	0.486	8.112	0.359	31	111	9	133	21	98 original
15576	90 [910; 9-(Z)-Hexadeceno	49 [877; Pyrophosphoric acid (4TMS)]	64	0.172	0.258	20.377	0.352	32	110	29	113	112	103 duplicate
8667	90 [910; 9-(Z)-Hexadeceno	140 [892; Ergosta-7,22-dien-3-ol (1TMS)]	49	0.168	0.392	16.800	0.369	33	109	17	125	86	85 original
8622	90 [910; 9-(Z)-Hexadeceno	95 [770; 3,4,6-Trisubstitutedphenylalanine (5TMS)]	50	0.166	0.238	19.859	0.352	34	108	30	112	109	104 original
8624	90 [910; 9-(Z)-Hexadeceno	97 [756; beta-D-Methylglucopyranoside (4TMS)]	52	0.155	0.162	19.524	0.392	35	107	35	107	104	64 original
8639	90 [910; 9-(Z)-Hexadeceno	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.153	0.161	17.261	0.372	38	108	36	106	92	82 original
8668	90 [910; 9-(Z)-Hexadeceno	139 [700; Ergosta-5,7-dien-3-ol]	38	0.141	0.316	19.342	0.453	37	105	23	119	103	12 original
15757	90 [910; 9-(Z)-Hexadeceno	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	0.140	0.099	19.860	0.335	38	104	46	96	107	128 duplicate
11506	90 [910; 9-(Z)-Hexadeceno	12 Glyceric acid	63	0.138	0.112	11.945	0.344	39	103	44	98	54	112 duplicate
15106	90 [910; 9-(Z)-Hexadeceno	44 [910; 2-Ketoglucuronic acid methoxyamine (4TMS)]	50	0.136	0.210	9.645	0.424	40	102	32	110	28	35 duplicate
12741	90 [910; 9-(Z)-Hexadeceno	22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.133	0.292	12.455	0.381	41	101	26	116	56	71 duplicate
8619	90 [910; 9-(Z)-Hexadeceno	92 [680; Glycerol-2-phosphate (4TMS)]	54	0.128	-0.231	10.595	0.367	42	100	115	27	38	86 original
14911	90 [910; 9-(Z)-Hexadeceno	42 Glutamic acid	60	0.121	0.013	26.914	0.334	43	99	72	70	127	129 duplicate
17624	90 [910; 9-(Z)-Hexadeceno	74 [912; Tetradecanoic acid (1TMS)]	64	0.114	0.073	11.190	0.393	44	98	52	90	47	61 duplicate
8662	90 [910; 9-(Z)-Hexadeceno	135	64	0.108	0.132	8.216	0.393	45	97	42	100	22	60 original
15667	90 [910; 9-(Z)-Hexadeceno	50 [746; Melibiose (8TMS); alpha-D-Gal(1,6)-D-Glc (8TMS)]	61	0.097	0.149	19.203	0.362	46	96	39	103	101	90 duplicate
16295	90 [910; 9-(Z)-Hexadeceno	85 [529; Ribonic acid-1,4-lactone (3TMS)]	48	0.092	0.090	4.369	0.360	47	95	48	94	2	85 duplicate
16595	90 [910; 9-(Z)-Hexadeceno	60 Glycerol-3-phosphate	64	0.089	0.101	17.552	0.434	48	94	45	97	93	26 duplicate
8649	90 [910; 9-(Z)-Hexadeceno	122 [644; Erythritol (4TMS)]	52	0.084	0.183	15.799	0.399	50	92	34	108	79	56 original
17134	90 [910; 9-(Z)-Hexadeceno	67 Citric acid	64	0.083	0.050	19.868	0.397	51	91	62	80	108	58 duplicate
8647	90 [910; 9-(Z)-Hexadeceno	120 [945; Uridine (3TMS)]	54	0.082	-0.024	9.370	0.342	52	90	80	62	26	116 original
8656	90 [910; 9-(Z)-Hexadeceno	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	59	0.080	0.059	12.719	0.441	53	89	55	87	57	17 original
11761	90 [910; 9-(Z)-Hexadeceno	14 Fumaric acid	64	0.072	0.079	9.977	0.370	54	88	51	91	29	84 duplicate
8629	90 [910; 9-(Z)-Hexadeceno	102 [904; Galactose methoxyamine (5TMS)]	64	0.060	0.086	7.213	0.347	55	87	50	92	15	110 original
8663	90 [910; 9-(Z)-Hexadeceno	138 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.059	-0.056	3.475	0.314	56	86	87	55	1	140 original
11634	90 [910; 9-(Z)-Hexadeceno	13 Uracil	64	0.059	0.043	13.718	0.400	57	85	66	76	65	65 duplicate
11377	90 [910; 9-(Z)-Hexadeceno	11 Succinic acid	64	0.053	-0.038	5.961	0.389	58	84	83	59	6	65 duplicate
8660	90 [910; 9-(Z)-Hexadeceno	133 [855; Squalene]	64	0.040	0.160	6.993	0.326	59	83	37	105	14	136 original
10309	90 [910; 9-(Z)-Hexadeceno	3 Ethanolamine	62	0.038	0.140	11.673	0.408	60	82	40	102	52	47 duplicate
17489	90 [910; 9-(Z)-Hexadeceno	72 [919; D-Xylopyranose (4TMS)]	63	0.036	-0.007	10.060	0.365	61	81	76	66	31	87 duplicate
18457	90 [910; 9-(Z)-Hexadeceno	88 Gluconic acid	64	0.036	0.047	10.937	0.416	62	80	65	77	45	44 duplicate
13207	90 [910; 9-(Z)-Hexadeceno	26 Citramalic acid	64	0.033	0.060	12.354	0.341	63	79	54	88	55	118 duplicate
15484	90 [910; 9-(Z)-Hexadeceno	48 Asparagine	64	0.028	0.137	10.765	0.434	64	78	41	101	42	27 duplicate
13434	90 [910; 9-(Z)-Hexadeceno	28 Malic acid	64	0.027	0.049	6.280	0.373	65	77	63	79	10	81 duplicate
12622	90 [910; 9-(Z)-Hexadeceno	21 [878; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	0.022	0.047	12.867	0.361	66	76	64	78	59	92 duplicate
14406	90 [910; 9-(Z)-Hexadeceno	37 Phenylalanine	64	0.021	0.009	18.861	0.377	67	75	73	69	99	75 duplicate
13546	90 [910; 9-(Z)-Hexadeceno	29 Erythritol	64	0.016	0.038	5.973	0.383	68	73	68	74	7	69 duplicate
15297	90 [910; 9-(Z)-Hexadeceno	46 Arabinose	64	0.016	-0.118	17.569	0.438	69	74	98	44	94	21 duplicate
16965	90 [910; 9-(Z)-Hexadeceno	65 [646; 3-Deoxyglucitol (5TMS)]	63	0.013	-0.043	15.813	0.442	70	72	85	57	80	16 duplicate
14611	90 [910; 9-(Z)-Hexadeceno	39 [829; 1-Phenylethanol (1TMS)]	63	0.012	0.052	15.105	0.377	71	71	61	81	74	74 duplicate
17207	90 [910; 9-(Z)-Hexadeceno	68 [570; Hypoxanthine (2TMS)]	20	0.011	0.055	15.877	0.429	72	70	59	83	82	30 duplicate
17819	90 [910; 9-(Z)-Hexadeceno	77 [826; beta-[[[5-methyl-2-thienyl)methyl]eneamino- benzeneacetic acid methyl ester]	62	0.009	-0.027	26.756	0.361	73	69	81	61	126	93 duplicate
8661	90 [910; 9-(Z)-Hexadeceno	134 Isomaltose	64	0.009	-0.067	23.050	0.434	74	68	89	53	117	25 original
15391	90 [910; 9-(Z)-Hexadeceno	47 [NA]	64	0.008	0.052	10.819	0.374	75	67	60	82	43	79 duplicate
8618	90 [910; 9-(Z)-Hexadeceno	91 [766; beta-D-Methylglucopyranoside (4TMS)]	64	0.001	0.087	17.112	0.330	76	66	49	93	89	135 original
18350	90 [910; 9-(Z)-Hexadeceno	86 [793; D-Galactono-1,4-lactone (4TMS)]	61	-0.002	-0.181	22.077	0.436	77	65	109	33	115	23 duplicate
12976	90 [910; 9-(Z)-Hexadeceno	24 [725; 2-Ketotartaric acid (2TMS)]	64	-0.003	-0.028	28.873	0.424	78	64	82	60	130	36 duplicate
16265	90 [910; 9-(Z)-Hexadeceno	56 [829; Orotic acid (3TMS)]	64	-0.006	-0.101	13.662	0.442	79	63	98	46	63	15 duplicate





8641	90 [910; 9-Z]-Hexadeceno	114	Fructose-6-phosphate	53	-0.234	-0.280	10.677	0.403	131	11	118	24	40	53 original
17060	90 [910; 9-Z]-Hexadeceno	66	Glyceric acid-3-phosphate	64	-0.262	-0.317	7.948	0.345	132	10	127	15	20	111 duplicate
8640	90 [910; 9-Z]-Hexadeceno	113	Galactose-6-phosphate	62	-0.263	-0.427	11.463	0.420	133	9	137	5	50	39 original
17690	90 [910; 9-Z]-Hexadeceno	75	Lysine	64	-0.284	-0.286	38.160	0.338	134	8	121	21	138	122 duplicate
8650	90 [910; 9-Z]-Hexadeceno	123	[945; Galactofuranose-6-phosphate (7TMS)]	64	-0.280	-0.445	8.670	0.462	135	7	139	3	24	11 original
8645	90 [910; 9-Z]-Hexadeceno	118	[928; Glucopyranose-6-phosphate (6TMS)]	58	-0.297	-0.432	10.845	0.374	136	6	138	4	44	78 original
13321	90 [910; 9-Z]-Hexadeceno	27	[915; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	-0.319	-0.283	20.058	0.336	137	5	120	22	110	126 duplicate
16432	90 [910; 9-Z]-Hexadeceno	58	[636; 4R-Acetylido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	-0.336	-0.331	13.780	0.333	138	4	129	13	66	132 duplicate
17944	90 [910; 9-Z]-Hexadeceno	79	Glucose	64	-0.387	-0.500	31.976	0.420	139	3	140	2	136	38 duplicate
11887	90 [910; 9-Z]-Hexadeceno	15	Alanine	64	-0.390	-0.556	16.278	0.406	140	2	141	1	85	51 duplicate
16909	90 [910; 9-Z]-Hexadeceno	64	[789; Tyramine (3TMS)]	63	-0.408	-0.372	6.434	0.357	141	1	132	10	11	99 duplicate
8674	91 [766; beta-D-Methylgluc	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	0.784	0.907	8.839	0.604	1	141	3	139	5	7 original
8680	91 [766; beta-D-Methylgluc	103	[648; Ethylamine (2TMS)]	63	0.733	0.909	7.243	0.640	2	140	2	140	1	1 original
8678	91 [766; beta-D-Methylgluc	101	[632; Dopamine (4TMS)]	64	0.694	0.924	8.555	0.624	3	139	1	141	3	3 original
8682	91 [766; beta-D-Methylgluc	105	[705; 2-Ketogluconic acid (5TMS)]	48	0.594	0.800	9.021	0.505	4	138	4	138	4	32 original
8711	91 [766; beta-D-Methylgluc	134	Isomaltose	64	0.585	0.713	20.027	0.492	5	137	9	133	68	40 original
8669	91 [766; beta-D-Methylgluc	92	[680; Glycerol-2-phosphate (4TMS)]	54	0.556	0.566	14.181	0.390	6	138	30	112	17	117 original
16268	91 [766; beta-D-Methylgluc	56	[829; Orolic acid (3TMS)]	64	0.551	0.710	13.810	0.501	7	135	10	132	15	36 duplicate
15288	91 [766; beta-D-Methylgluc	46	Arabinose	64	0.549	0.702	13.469	0.498	8	134	11	131	13	37 duplicate
11635	91 [766; beta-D-Methylgluc	13	Uracil	64	0.548	0.729	14.687	0.525	9	133	6	136	21	18 duplicate
16986	91 [766; beta-D-Methylgluc	65	[646; 3-Deoxyglucitol (5TMS)]	63	0.545	0.680	14.240	0.481	10	132	15	127	18	50 duplicate
8676	91 [766; beta-D-Methylgluc	99	[662; Ribose-5-phosphate methoxamine (BP) (5TMS)]	41	0.532	0.684	16.798	0.442	11	131	14	128	35	82 original
18458	91 [766; beta-D-Methylgluc	88	Gluconic acid	64	0.513	0.685	12.709	0.511	12	130	13	129	10	26 duplicate
12013	91 [766; beta-D-Methylgluc	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	0.506	0.716	17.143	0.522	13	129	8	134	39	18 duplicate
8706	91 [766; beta-D-Methylgluc	129	[840; Maltose methoxamine (6TMS); alpha-D-Glc-(1,4)-D-Glc	59	0.500	0.665	13.045	0.444	14	128	20	122	12	80 original
12977	91 [766; beta-D-Methylgluc	24	[725; 2-Ketocacanic acid (2TMS)]	64	0.494	0.700	28.865	0.511	15	127	12	130	117	27 duplicate
12137	91 [766; beta-D-Methylgluc	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	0.489	0.678	16.591	0.468	16	128	16	128	32	59 duplicate
18351	91 [766; beta-D-Methylgluc	86	[783; D-Galactono-1,4-lactone (4TMS)]	61	0.479	0.638	17.627	0.484	17	125	23	119	49	48 duplicate
16350	91 [766; beta-D-Methylgluc	57	[757; 2-Desoxy-pentos-3-ylose dimethoxamine (2TMS)]	55	0.471	0.630	12.797	0.400	18	124	24	118	11	113 duplicate
14612	91 [766; beta-D-Methylgluc	39	[828; 1-Phenylethanol (1TMS)]	63	0.471	0.655	14.004	0.435	19	123	21	121	16	89 duplicate
16022	91 [766; beta-D-Methylgluc	54	[NA]	55	0.452	0.673	17.009	0.398	20	122	18	124	36	115 duplicate
15668	91 [766; beta-D-Methylgluc	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	0.445	0.672	24.321	0.454	21	121	19	123	97	73 duplicate
16755	91 [766; beta-D-Methylgluc	62	[812; D-Xylofuranose (4TMS)]	64	0.443	0.610	16.743	0.435	22	120	26	116	33	90 duplicate
10033	91 [766; beta-D-Methylgluc	1	[938; Sulfuric acid (2TMS)]	36	0.438	0.723	13.771	0.471	23	119	7	135	14	56 duplicate
13547	91 [766; beta-D-Methylgluc	29	Erythritol	64	0.434	0.676	15.590	0.479	24	118	17	125	26	51 duplicate
11378	91 [766; beta-D-Methylgluc	11	Succinic acid	64	0.411	0.605	14.922	0.436	25	117	27	115	24	86 duplicate
14510	91 [766; beta-D-Methylgluc	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.404	0.623	14.419	0.451	26	116	25	117	19	75 duplicate
18405	91 [766; beta-D-Methylgluc	87	[945; beta-D-Glucopyranose (5TMS)]	62	0.401	0.528	32.219	0.421	27	115	34	108	128	97 duplicate
8705	91 [766; beta-D-Methylgluc	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.370	0.544	12.488	0.382	28	114	32	110	9	120 original
12742	91 [766; beta-D-Methylgluc	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.354	0.592	17.412	0.437	29	113	28	114	44	87 duplicate
15392	91 [766; beta-D-Methylgluc	47	[NA]	64	0.354	0.535	14.571	0.457	30	112	33	109	20	68 duplicate
11762	91 [766; beta-D-Methylgluc	14	Fumaric acid	64	0.339	0.565	17.880	0.443	31	111	31	111	51	81 duplicate
11507	91 [766; beta-D-Methylgluc	12	Glycemic acid	63	0.330	0.567	19.024	0.412	32	110	29	113	57	103 duplicate
8683	91 [766; beta-D-Methylgluc	106	[733; Threitol (4TMS)]	62	0.314	0.390	15.934	0.583	33	109	45	97	28	10 original
17351	91 [766; beta-D-Methylgluc	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	0.313	0.385	19.699	0.433	34	108	47	95	65	92 duplicate
8692	91 [766; beta-D-Methylgluc	115	Glucose-6-phosphate	62	0.310	0.461	23.486	0.454	35	107	39	103	90	72 original
13435	91 [766; beta-D-Methylgluc	28	Malic acid	64	0.300	0.515	15.566	0.451	36	106	35	107	25	76 duplicate
18006	91 [766; beta-D-Methylgluc	80	[772; D-Glucose (5TMS)]	62	0.287	0.460	27.729	0.409	37	105	40	102	113	105 duplicate

17883	91 [766; beta-D-Methylgluc	78	Mannose	62	0.285	0.389	17.316	0.420	39	103	46	96	40	98 duplicate
17756	91 [766; beta-D-Methylgluc	76	Fructose	64	0.272	0.480	23.442	0.448	40	102	36	106	89	79 duplicate
10718	91 [766; beta-D-Methylgluc	6	Glycerol	84	0.263	0.480	39.640	0.449	41	101	43	99	139	77 duplicate
8670	91 [766; beta-D-Methylgluc	93	[607; Putrescine (4TMS)]	60	0.262	0.648	20.328	0.462	42	100	22	120	71	65 original
12623	91 [766; beta-D-Methylgluc	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	0.261	0.397	18.762	0.405	43	99	44	98	58	109 duplicate
13208	91 [766; beta-D-Methylgluc	26	Citramalic acid	64	0.250	0.376	19.276	0.412	44	98	50	92	61	102 duplicate
14198	91 [766; beta-D-Methylgluc	35	Pyroglutamic acid	64	0.244	0.461	38.964	0.463	45	97	38	104	138	63 duplicate
8689	91 [766; beta-D-Methylgluc	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.238	0.369	24.165	0.440	46	96	51	91	98	84 original
8704	91 [766; beta-D-Methylgluc	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.236	0.383	14.874	0.271	47	95	48	94	23	141 original
14713	91 [766; beta-D-Methylgluc	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.234	0.342	33.412	0.456	48	94	52	90	130	70 duplicate
17558	91 [766; beta-D-Methylgluc	73	[608; Glucose methoxyamine (5TMS)]	57	0.232	0.224	16.513	0.482	49	93	58	84	31	66 duplicate
8702	91 [766; beta-D-Methylgluc	125	[882; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	0.227	0.477	29.142	0.459	50	92	37	105	120	67 original
8677	91 [766; beta-D-Methylgluc	100	[857; Mannitol (6TMS)]	64	0.213	0.383	15.921	0.414	51	91	49	93	27	101 original
8697	91 [766; beta-D-Methylgluc	120	[945; Uridine (3TMS)]	54	0.212	0.188	16.123	0.407	52	90	62	80	30	108 original
8694	91 [766; beta-D-Methylgluc	117	[724; Glycerol (3TMS)]	56	0.187	0.203	17.688	0.437	53	89	61	81	50	86 original
8679	91 [766; beta-D-Methylgluc	102	[904; Galactose methoxyamine (5TMS)]	64	0.182	0.303	17.378	0.380	54	88	54	88	42	122 original
18240	91 [766; beta-D-Methylgluc	84	Mannitol	62	0.179	0.768	26.267	0.548	55	87	5	137	105	13 duplicate
11888	91 [766; beta-D-Methylgluc	15	Alanine	64	0.157	0.186	20.580	0.488	56	86	63	79	74	45 duplicate
8712	91 [766; beta-D-Methylgluc	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	0.145	0.222	17.591	0.383	57	85	59	83	47	119	original
8697	91 [766; beta-D-Methylgluc	110	[715; Erythritol (4TMS)]	54	0.136	0.216	19.683	0.502	58	84	60	82	64	34 original
8691	91 [766; beta-D-Methylgluc	114	Fructose-6-phosphate	53	0.122	0.261	18.223	0.550	59	83	55	87	53	11 original
8698	91 [766; beta-D-Methylgluc	121	[657; Erythritol (4TMS)]	55	0.118	0.099	22.938	0.404	60	82	69	73	84	110 original
8690	91 [766; beta-D-Methylgluc	113	Galactose-6-phosphate	62	0.117	0.328	17.488	0.502	61	81	53	89	45	33 original
16910	91 [766; beta-D-Methylgluc	64	[789; Tyramine (3TMS)]	63	0.114	0.121	17.370	0.358	62	80	67	75	41	130 duplicate
17945	91 [766; beta-D-Methylgluc	78	Glucose	64	0.104	0.252	33.378	0.535	63	79	56	86	129	16 duplicate
8709	91 [766; beta-D-Methylgluc	132	[895; Isomaltose methoxyamine (8TMS)]	42	0.103	0.435	20.745	0.338	64	78	41	101	76	138 original
15010	91 [766; beta-D-Methylgluc	43	[548; Leucine (2TBS)]	60	0.103	0.102	15.974	0.441	65	77	68	74	29	83 duplicate
12382	91 [766; beta-D-Methylgluc	19	Alanine (BP) (3TMS)	64	0.098	0.175	17.528	0.481	66	76	64	78	46	49 duplicate
8699	91 [766; beta-D-Methylgluc	122	[644; Erythritol (4TMS)]	52	0.097	0.236	23.242	0.428	67	75	57	85	88	94 original
12260	91 [766; beta-D-Methylgluc	18	[590; 1-Acetyl-2-thiohydantoin]	64	0.086	0.073	17.041	0.367	68	74	72	70	37	127 duplicate
14813	91 [766; beta-D-Methylgluc	41	[639; Proline (2TMS)]	64	0.077	0.046	18.704	0.466	69	73	75	67	55	61 duplicate
8673	91 [766; beta-D-Methylgluc	96	myo-Inositol	49	0.077	0.029	22.252	0.426	70	72	77	65	82	96 original
8700	91 [766; beta-D-Methylgluc	123	[945; Galactofuranose-6-phosphate (7TMS)]	64	0.070	0.041	17.622	0.548	71	71	76	66	48	14 original
8688	91 [766; beta-D-Methylgluc	111	[583; Erythritol (4TMS)]	42	0.068	0.058	25.530	0.329	72	70	73	69	100	138 original
8681	91 [766; beta-D-Methylgluc	104	[795; Erythritol (4TMS)]	63	0.061	-0.026	18.073	0.465	73	69	81	61	52	62 original
18296	91 [766; beta-D-Methylgluc	85	[528; Methylcitric acid (4TMS)]	48	0.046	0.132	8.489	0.508	74	68	66	76	2	29 duplicate
8693	91 [766; beta-D-Methylgluc	116	[882; Pseudouridine (5TMS)]	30	0.044	-0.020	10.007	0.492	75	67	79	63	6	41 original
15935	91 [766; beta-D-Methylgluc	53	Glycerol-2-phosphate	64	0.035	0.145	20.304	0.355	76	66	65	77	70	131 duplicate
15107	91 [766; beta-D-Methylgluc	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	0.025	0.092	17.409	0.427	77	65	70	72	43	95 duplicate
17625	91 [766; beta-D-Methylgluc	74	[912; Tetradecanoic acid (1TMS)]	64	0.020	-0.023	20.413	0.456	78	64	80	62	72	69 duplicate
8695	91 [766; beta-D-Methylgluc	118	[928; Glucopyranose-6-phosphate (6TMS)]	58	0.004	0.057	19.122	0.352	79	63	74	68	59	132 original
18361	91 [766; beta-D-Methylgluc	90	[910; 9-(Z)-Hexadecanoic acid (1TMS)]	64	0.001	0.087	17.112	0.330	80	62	71	71	38	137 duplicate
17490	91 [766; beta-D-Methylgluc	72	[918; D-Xylopyranose (4TMS)]	63	-0.011	0.017	18.295	0.369	81	61	78	64	62	126 duplicate
8717	91 [766; beta-D-Methylgluc	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	49	-0.054	-0.066	19.377	0.433	82	60	83	59	63	91 original
8713	91 [766; beta-D-Methylgluc	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.074	-0.302	10.744	0.300	83	59	94	48	7	140 original
8703	91 [766; beta-D-Methylgluc	126	[559; Erythritol (4TMS)]	45	-0.089	-0.178	19.756	0.439	84	58	85	57	66	85 original
15577	91 [766; beta-D-Methylgluc	49	[877; Pyrophosphoric acid (4TMS)]	64	-0.095	-0.027	27.558	0.366	85	57	82	60	112	128 duplicate
13093	91 [766; beta-D-Methylgluc	25	[709; 2,5-Diaminvalerolactam (2TMS)]	48	-0.099	-0.415	26.306	0.409	86	56	101	41	106	104 duplicate
8716	91 [766; beta-D-Methylgluc	139	[700; Ergosta-5,7-dien-3-ol]	38	-0.124	-0.205	21.995	0.319	87	55	88	54	80	139 original
8710	91 [766; beta-D-Methylgluc	133	[855; Squalene]	64	-0.138	-0.392	20.227	0.401	88	54	98	44	69	112 original

8715	91 [766; beta-D-Methylgluc 138 [674; Ergosterol (1TMS)]	46 -0.144	-0.413	23,509	0.522	89	53	100	42	92	20 original
18183	91 [766; beta-D-Methylgluc 83 Sorbitol	58 -0.145	-0.582	26,351	0.530	90	52	115	27	107	17 duplicate
10447	91 [766; beta-D-Methylgluc 4 Phosphoric acid	52 -0.150	-0.549	35,972	0.471	91	51	114	28	138	57 duplicate
16833	91 [766; beta-D-Methylgluc 3 Glutamine	52 -0.152	-0.411	27,015	0.506	92	50	99	43	110	31 duplicate
15203	91 [766; beta-D-Methylgluc 45 Homocysteine	61 -0.158	-0.139	28,903	0.375	93	49	84	58	118	123 duplicate
8684	91 [766; beta-D-Methylgluc 107 9-(Z)-Octadecenoic acid	64 -0.164	-0.230	19,802	0.345	94	48	89	53	67	134 original
8686	91 [766; beta-D-Methylgluc 109 Octadecanoic acid	64 -0.191	-0.277	27,397	0.374	95	47	93	49	111	124 original
13322	91 [766; beta-D-Methylgluc 27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53 -0.192	-0.587	26,375	0.448	96	46	116	26	108	78 duplicate
8696	91 [766; beta-D-Methylgluc 119 [931; myo-Inositol-2-phosphate (7TMS)]	64 -0.201	-0.188	19,102	0.339	97	45	87	55	58	135 original
8718	91 [766; beta-D-Methylgluc 141 Lanosta-8,24-dien-3-beta-ol	61 -0.216	-0.269	22,058	0.387	98	44	91	51	81	118 original
16433	91 [766; beta-D-Methylgluc 58 (1TMS)]	64 -0.218	-0.643	23,986	0.507	99	43	123	19	95	30 duplicate
8675	91 [766; beta-D-Methylgluc 98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	48 -0.222	-0.520	28,114	0.510	100	42	111	31	115	28 original
15847	91 [766; beta-D-Methylgluc 52 [NA]	46 -0.225	-0.390	29,989	0.603	101	41	97	45	122	8 duplicate
8671	91 [766; beta-D-Methylgluc 94 Hexadecanoic acid	64 -0.230	-0.326	25,762	0.407	102	40	95	47	103	107 original
18125	91 [766; beta-D-Methylgluc 82 Lysine	39 -0.231	-0.418	21,464	0.613	103	39	102	40	77	4 duplicate
10583	91 [766; beta-D-Methylgluc 5 Leucine	45 -0.236	-0.186	11,845	0.521	104	38	86	56	8	22 duplicate
16876	91 [766; beta-D-Methylgluc 61 [NA]	64 -0.243	-0.275	18,416	0.400	105	37	92	50	54	114 duplicate
8672	91 [766; beta-D-Methylgluc 95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50 -0.246	-0.347	28,254	0.467	106	36	96	46	116	60 original
17681	91 [766; beta-D-Methylgluc 75 Lysine	64 -0.251	-0.699	40,180	0.502	107	35	129	13	140	35 duplicate
10985	91 [766; beta-D-Methylgluc 8 Isoleucine	55 -0.254	-0.691	26,975	0.472	108	34	127	15	109	55 duplicate
10172	91 [766; beta-D-Methylgluc 2 Serine	62 -0.258	-0.720	29,090	0.473	109	33	132	10	119	53 duplicate
12860	91 [766; beta-D-Methylgluc 23 Homoserine	64 -0.266	-0.536	23,155	0.484	110	32	112	30	87	46 duplicate
8707	91 [766; beta-D-Methylgluc 130 Trehalose	63 -0.267	-0.476	30,423	0.403	111	31	105	37	123	111 original
8708	91 [766; beta-D-Methylgluc 131 [626; 5-Methylthiadenosine (3TMS)]	55 -0.273	-0.231	23,805	0.487	112	30	90	52	94	44 original
18510	91 [766; beta-D-Methylgluc 89 [775; Dopamine (4TMS)]	35 -0.284	-0.465	21,690	0.611	113	29	103	39	78	5 duplicate
8701	91 [766; beta-D-Methylgluc 124 [734; 1-Monoleoylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	59 -0.305	-0.498	30,786	0.369	114	28	110	32	125	125 original
8714	91 [766; beta-D-Methylgluc 137 Ergosterol	64 -0.315	-0.493	23,488	0.349	115	27	108	34	91	133 original
15758	91 [766; beta-D-Methylgluc 51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44 -0.317	-0.548	22,895	0.514	116	26	113	29	83	24 duplicate
8685	91 [766; beta-D-Methylgluc 108 Octadecanoic acid	64 -0.319	-0.494	20,642	0.380	117	25	109	33	75	121 original
15485	91 [766; beta-D-Methylgluc 48 Asparagine	64 -0.320	-0.473	23,768	0.489	118	24	104	38	93	43 duplicate
14092	91 [766; beta-D-Methylgluc 34 Aspartic acid	64 -0.331	-0.480	34,338	0.393	119	23	106	36	132	116 duplicate
13985	91 [766; beta-D-Methylgluc 33 Methionine	64 -0.346	-0.482	22,946	0.414	120	22	107	35	85	100 duplicate
17208	91 [766; beta-D-Methylgluc 68 [570; Hypoxanthine (2TMS)]	20 -0.347	-0.685	16,777	0.568	121	21	126	16	34	9 duplicate
12503	91 [766; beta-D-Methylgluc 20 [619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31 -0.359	-0.626	14,844	0.625	122	20	121	21	22	2 duplicate
17280	91 [766; beta-D-Methylgluc 69 Arginine	60 -0.362	-0.591	27,824	0.463	123	19	119	23	114	64 duplicate
10852	91 [766; beta-D-Methylgluc 7 Threonine	64 -0.377	-0.705	31,360	0.473	124	18	130	12	126	54 duplicate
11117	91 [766; beta-D-Methylgluc 9 Proline	63 -0.380	-0.751	35,144	0.493	125	17	136	6	133	39 duplicate
13768	91 [766; beta-D-Methylgluc 31 [622; Parabanic acid (2TMS)]	64 -0.382	-0.618	23,063	0.433	126	16	120	22	86	83 duplicate
14303	91 [766; beta-D-Methylgluc 36 [596; N-Acetylglutamic acid (2TMS)]	64 -0.387	-0.803	31,998	0.522	127	15	140	2	127	21 duplicate
16108	91 [766; beta-D-Methylgluc 55 [612; 4-Aminobutyric acid (2TBS)]	43 -0.389	-0.581	21,740	0.550	128	14	118	24	79	12 duplicate
13877	91 [766; beta-D-Methylgluc 32 [728; N,N-Dimethyllysine methyl ester]	63 -0.393	-0.708	29,591	0.511	129	13	131	11	121	25 duplicate
17061	91 [766; beta-D-Methylgluc 66 Glycine acid-3-phosphate	64 -0.394	-0.764	20,494	0.493	130	12	137	5	73	38 duplicate
17421	91 [766; beta-D-Methylgluc 71 [731; Erythrose (3TMS)]	64 -0.397	-0.640	19,217	0.491	131	11	122	20	60	42 duplicate
16515	91 [766; beta-D-Methylgluc 59 Ornithine; Arginine	64 -0.406	-0.678	41,324	0.453	132	10	125	17	141	74 duplicate
13658	91 [766; beta-D-Methylgluc 30 [815; Ethyl-3(2H)-thiophenone]	64 -0.416	-0.580	33,578	0.408	133	9	117	25	131	106 duplicate
11248	91 [766; beta-D-Methylgluc 10 Glycine	64 -0.438	-0.843	25,650	0.484	134	8	124	18	102	47 duplicate
17820	91 [766; beta-D-Methylgluc 77 benzeneacetic acid methyl ester]	62 -0.443	-0.726	35,353	0.477	135	7	135	7	134	52 duplicate

14407	91 [766; beta-D-Methylgluc	37	Phenylalanine	64	-0.466	-0.722	25.581	0.469	136	6	134	8	101	58 duplicate
10310	91 [766; beta-D-Methylgluc	3	Ethanolamine	82	-0.474	-0.722	24.364	0.544	137	5	133	9	88	15 duplicate
14912	91 [766; beta-D-Methylgluc	42	Glutamic acid	60	-0.477	-0.697	35.924	0.455	138	4	128	14	135	71 duplicate
18066	91 [766; beta-D-Methylgluc	81	Tyrosine	84	-0.518	-0.830	37.948	0.608	139	3	141	1	137	6 duplicate
16596	91 [766; beta-D-Methylgluc	60	Glycerol-3-phosphate	84	-0.523	-0.778	25.529	0.514	140	2	139	3	99	23 duplicate
17135	91 [766; beta-D-Methylgluc	67	Citric acid	84	-0.549	-0.771	25.949	0.419	141	1	138	4	104	99 duplicate
8729	92 [680; Glycerol-2-phosph	103	[648; Ethylamine (2TMS)]	53	0.769	0.675	11.056	0.466	1	141	34	108	46	66 original
8731	92 [680; Glycerol-2-phosph	105	[705; 2-Ketogluconic acid (5TMS)]	48	0.762	0.896	8.914	0.534	2	140	1	141	30	39 original
8760	92 [680; Glycerol-2-phosph	134	Isomaltose	54	0.753	0.839	22.865	0.619	3	139	12	130	118	2 original
8723	92 [680; Glycerol-2-phosph	97	[756; beta-D-Methylglucopyranoside (4TMS)]	50	0.683	0.797	16.623	0.519	4	138	14	128	86	47 original
16351	92 [680; Glycerol-2-phosph													
16987	92 [680; Glycerol-2-phosph	65	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	51	0.680	0.872	8.413	0.617	5	137	6	136	24	4 duplicate
16336	92 [680; Glycerol-2-phosph	13	[646; 3-Deoxyglucitol (5TMS)]	53	0.678	0.807	6.437	0.618	6	136	13	129	6	3 duplicate
15299	92 [680; Glycerol-2-phosph	46	Arabinose	54	0.676	0.760	14.628	0.561	7	135	21	121	68	22 duplicate
16267	92 [680; Glycerol-2-phosph	56	[829; Orotic acid (3TMS)]	54	0.667	0.882	13.479	0.613	8	133	4	138	60	5 duplicate
18459	92 [680; Glycerol-2-phosph	88	Gluconic acid	54	0.667	0.850	4.701	0.604	9	134	9	133	3	9 duplicate
		129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	54	0.645	0.713	10.330	0.562	10	132	26	116	37	21 duplicate
8755	92 [680; Glycerol-2-phosph													
12014	92 [680; Glycerol-2-phosph	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	52	0.643	0.789	6.539	0.585	11	131	16	126	7	12 original
12978	92 [680; Glycerol-2-phosph	24	[725; 2-Ketooctanoic acid (2TMS)]	54	0.642	0.745	16.449	0.561	12	130	23	119	85	23 duplicate
8754	92 [680; Glycerol-2-phosph	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	54	0.637	0.785	29.908	0.611	13	129	19	123	130	7 duplicate
16023	92 [680; Glycerol-2-phosph	54	[NA]	45	0.634	0.853	4.438	0.582	14	128	8	134	2	15 original
8727	92 [680; Glycerol-2-phosph	101	[832; Dopamine (4TMS)]	52	0.618	0.788	7.679	0.522	15	127	17	125	15	45 duplicate
15669	92 [680; Glycerol-2-phosph	50	[748; Ribonic acid-1,4-lactone (3TMS)]	54	0.616	0.635	8.800	0.395	16	128	38	104	29	93 original
16756	92 [680; Glycerol-2-phosph	62	[812; D-Xylofuranose (4TMS)]	53	0.604	0.708	15.110	0.506	17	125	29	113	74	52 duplicate
18352	92 [680; Glycerol-2-phosph	86	[793; D-Galactono-1,4-lactone (4TMS)]	54	0.600	0.791	13.515	0.583	18	124	15	127	62	14 duplicate
13548	92 [680; Glycerol-2-phosph	29	Erythritol	51	0.600	0.894	17.941	0.605	19	123	2	140	92	8 duplicate
14613	92 [680; Glycerol-2-phosph	39	[829; 1-Phenylethanol (1TMS)]	54	0.586	0.689	7.154	0.501	20	122	32	110	11	53 duplicate
12138	92 [680; Glycerol-2-phosph	17	[700; 2-methyl-1,2-propanediol (2TMS)]	53	0.582	0.713	13.646	0.532	21	121	25	117	64	40 duplicate
8725	92 [680; Glycerol-2-phosph	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	54	0.575	0.749	16.108	0.497	22	120	22	120	83	55 duplicate
14511	92 [680; Glycerol-2-phosph	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	39	0.571	0.686	8.173	0.558	23	119	33	109	20	27 original
18612	92 [680; Glycerol-2-phosph	91	[766; beta-D-Methylglucopyranoside (4TMS)]	54	0.568	0.711	7.761	0.540	24	118	28	114	16	37 duplicate
11379	92 [680; Glycerol-2-phosph	11	Succinic acid	54	0.556	0.566	14.181	0.390	25	117	47	95	66	95 duplicate
18287	92 [680; Glycerol-2-phosph	85	[529; Methylcitric acid (4TMS)]	38	0.531	0.712	8.161	0.496	26	116	27	115	19	56 duplicate
11763	92 [680; Glycerol-2-phosph	14	Fumaric acid	54	0.500	0.653	8.250	0.478	28	114	36	106	22	117 duplicate
11508	92 [680; Glycerol-2-phosph	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	54	0.493	0.576	8.705	0.491	29	113	48	96	35	59 duplicate
12743	92 [680; Glycerol-2-phosph	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	47	0.488	0.611	17.570	0.514	30	112	40	102	90	49 duplicate
8753	92 [680; Glycerol-2-phosph	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	45	0.481	0.587	9.455	0.518	31	111	44	98	33	48 duplicate
8719	92 [680; Glycerol-2-phosph	93	[607; Putrescine (4TMS)]	39	0.471	0.545	4.854	0.581	32	110	50	92	4	16 original
13436	92 [680; Glycerol-2-phosph	28	Malic acid	51	0.467	0.243	15.299	0.368	33	109	74	68	76	103 original
8741	92 [680; Glycerol-2-phosph	115	Glucose-6-phosphate	54	0.458	0.639	9.576	0.488	34	108	37	105	34	60 duplicate
8726	92 [680; Glycerol-2-phosph	100	[857; Mannitol (6TMS)]	53	0.451	0.850	23.217	0.612	35	107	10	132	119	6 original
8732	92 [680; Glycerol-2-phosph	106	[733; Threitol (4TMS)]	54	0.434	0.478	9.426	0.460	37	106	56	86	32	69 original
17894	92 [680; Glycerol-2-phosph	78	Mannose	52	0.415	0.704	8.702	0.553	38	104	30	112	27	33 original
8738	92 [680; Glycerol-2-phosph	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	53	0.392	0.665	6.734	0.551	39	103	35	107	9	35 duplicate
17757	92 [680; Glycerol-2-phosph	76	Fructose	52	0.398	0.425	14.860	0.427	40	102	62	80	69	81 original
14714	92 [680; Glycerol-2-phosph	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	54	0.378	0.875	23.689	0.595	41	101	5	137	120	11 duplicate
14199	92 [680; Glycerol-2-phosph	35	Pyroglutamic acid	54	0.375	0.584	31.860	0.454	42	100	45	97	134	73 duplicate
				54	0.375	0.864	38.523	0.557	43	99	7	135	140	28 duplicate

8761	92 [680; Glycerol-2-phosph	135	54	0.372	0.316	12.373	0.390	44	98	69	73	54	94 original
13209	92 [680; Glycerol-2-phosph		54	0.370	0.507	15.700	0.435	45	97	54	88	78	78 duplicate
12624	92 [680; Glycerol-2-phosph		54	0.368	0.526	15.682	0.456	46	96	51	91	77	71 duplicate
8728	92 [680; Glycerol-2-phosph		54	0.367	0.382	8.211	0.467	47	95	64	78	21	64 original
10034	92 [680; Glycerol-2-phosph		50	0.365	0.525	7.471	0.513	48	94	52	90	13	50 original
18241	92 [680; Glycerol-2-phosph		36	0.340	0.608	6.996	0.558	49	93	41	101	10	26 duplicate
17559	92 [680; Glycerol-2-phosph		52	0.335	0.372	28.732	0.404	50	92	66	76	129	88 duplicate
8746	92 [680; Glycerol-2-phosph		47	0.332	0.594	7.514	0.434	51	91	43	99	14	79 duplicate
8736	92 [680; Glycerol-2-phosph		49	0.332	0.176	11.643	0.488	52	90	75	67	50	61 original
8748	92 [680; Glycerol-2-phosph		49	0.330	0.546	8.500	0.598	53	89	49	93	25	10 original
8747	92 [680; Glycerol-2-phosph		49	0.301	0.508	13.416	0.524	54	87	53	89	59	43 original
18406	92 [680; Glycerol-2-phosph		49	0.301	0.427	11.784	0.521	55	88	61	81	53	46 original
15108	92 [680; Glycerol-2-phosph		52	0.288	0.849	33.145	0.570	56	88	11	131	136	18 duplicate
8752	92 [680; Glycerol-2-phosph		24	0.275	0.099	9.714	0.387	57	85	78	64	36	96 original
8752	92 [680; Glycerol-2-phosph		48	0.241	0.381	7.916	0.559	58	84	65	77	17	25 duplicate
15993	92 [680; Glycerol-2-phosph		45	0.238	0.260	8.551	0.553	59	83	72	70	26	32 original
12261	92 [680; Glycerol-2-phosph		54	0.224	0.258	10.654	0.464	60	82	73	69	40	67 duplicate
8739	92 [680; Glycerol-2-phosph		54	0.220	0.894	30.111	0.545	61	81	3	139	131	36 original
17626	92 [680; Glycerol-2-phosph		54	0.201	0.394	8.960	0.387	62	80	63	79	31	97 duplicate
18007	92 [680; Glycerol-2-phosph		39	0.201	0.560	12.500	0.555	63	79	48	94	55	28 original
18562	92 [680; Glycerol-2-phosph		53	0.183	0.785	5.690	0.551	64	78	18	124	5	34 original
8745	92 [680; Glycerol-2-phosph		52	0.145	0.283	10.788	0.358	65	77	71	71	43	109 duplicate
8737	92 [680; Glycerol-2-phosph		54	0.128	0.765	28.628	0.527	66	76	20	122	127	41 duplicate
10719	92 [680; Glycerol-2-phosph		54	0.111	-0.231	11.595	0.367	67	75	90	52	39	104 duplicate
8722	92 [680; Glycerol-2-phosph		54	0.104	-0.318	11.770	0.455	68	74	97	45	52	72 original
18184	92 [680; Glycerol-2-phosph		39	0.099	0.099	18.616	0.400	69	73	79	63	94	81 original
8766	92 [680; Glycerol-2-phosph		54	0.099	0.722	39.061	0.553	70	72	24	118	141	31 duplicate
12383	92 [680; Glycerol-2-phosph		39	0.096	0.122	16.114	0.247	71	71	77	65	84	137 original
8735	92 [680; Glycerol-2-phosph		39	0.089	0.011	13.801	0.331	72	70	81	61	65	121 original
14814	92 [680; Glycerol-2-phosph		48	0.089	-0.168	20.937	0.261	73	69	89	53	108	136 duplicate
8740	92 [680; Glycerol-2-phosph		51	0.089	-0.107	14.247	0.365	74	68	86	56	67	106 original
16834	92 [680; Glycerol-2-phosph		54	0.082	0.600	11.433	0.523	75	66	42	100	49	44 duplicate
8730	92 [680; Glycerol-2-phosph		54	0.082	0.135	22.090	0.428	76	67	76	66	116	80 original
8720	92 [680; Glycerol-2-phosph		54	0.075	0.427	13.409	0.442	77	65	60	82	58	77 duplicate
8733	92 [680; Glycerol-2-phosph		45	0.071	0.692	6.552	0.581	78	64	31	111	8	17 original
15938	92 [680; Glycerol-2-phosph		42	0.064	-0.757	19.313	0.628	79	63	133	9	97	1 duplicate
8759	92 [680; Glycerol-2-phosph		53	0.051	0.361	8.756	0.448	80	62	67	75	28	75 original
8749	92 [680; Glycerol-2-phosph		54	0.048	0.055	20.954	0.408	81	60	80	62	108	87 original
15848	92 [680; Glycerol-2-phosph		54	0.048	-0.399	14.900	0.397	82	61	105	37	71	92 original
17491	92 [680; Glycerol-2-phosph		54	0.036	-0.065	11.723	0.318	83	59	84	58	51	127 duplicate
8762	92 [680; Glycerol-2-phosph		31	0.019	-0.249	18.100	0.381	84	58	93	49	82	98 original
8744	92 [680; Glycerol-2-phosph		54	0.012	-0.011	10.697	0.298	85	57	82	60	42	132 original
16911	92 [680; Glycerol-2-phosph		54	-0.006	0.443	11.321	0.447	86	56	59	83	47	76 original
17422	92 [680; Glycerol-2-phosph		36	-0.008	-0.706	21.962	0.554	87	55	131	11	115	30 duplicate
			53	-0.010	-0.024	10.952	0.363	88	54	83	59	44	107 duplicate
			54	-0.023	-0.246	15.815	0.376	89	53	92	50	81	100 original
			17	-0.029	-0.148	3.757	0.466	90	52	87	55	1	65 original
			50	-0.081	0.327	7.977	0.495	91	51	68	74	18	57 original
			54	-0.086	0.210	8.319	0.421	92	50	70	72	23	83 duplicate
			54	-0.132	-0.237	12.638	0.353	93	49	91	51	56	113 duplicate

92 [680; Glycerol-2-phosph	43 [548; Leucine (2TBS)]	50 -0.135	-0.155	10.981	0.280	94	48	88	54	45	134
92 [680; Glycerol-2-phosph	138 [674; Ergosterol (1TMS)]	36 -0.137	-0.081	14.872	0.410	95	47	85	57	70	86
92 [680; Glycerol-2-phosph	15 Alanine	54 -0.154	0.445	17.919	0.564	96	46	58	84	91	20
124 [734; 1-Monoooleylglycerol (2TMS); 1-											
92 [680; Glycerol-2-phosph	Monohexadecenoyle/glycerol (1TMS)]	49 -0.156	-0.337	21.852	0.373	97	45	99	43	113	102
92 [680; Glycerol-2-phosph	61 [NA]	54 -0.163	-0.507	10.487	0.463	98	44	116	26	38	68
92 [680; Glycerol-2-phosph	95 [770; 3,4,8-Trisubhydroxyphenylethanamine (5TMS)]	54 -0.179	-0.544	19.740	0.323	99	43	119	23	99	125
92 [680; Glycerol-2-phosph	49 [877; Pyrophosphoric acid (4TMS)]	54 -0.210	-0.460	21.957	0.402	100	42	111	31	114	90
92 [680; Glycerol-2-phosph	89 [775; Dopamine (4TMS)]	25 -0.213	-0.906	19.466	0.509	101	41	139	3	98	51
92 [680; Glycerol-2-phosph	108 Octadecanoic acid	54 -0.223	-0.410	11.341	0.378	102	40	107	35	48	99
92 [680; Glycerol-2-phosph	79 Glucose	54 -0.234	0.617	33.343	0.568	103	39	103	137	19	19
92 [680; Glycerol-2-phosph	45 Homocysteine	51 -0.236	-0.347	20.696	0.323	104	38	101	41	104	126
92 [680; Glycerol-2-phosph	25 [709; 2,5-Diaminovalerolactam (2TMS)]	46 -0.287	-0.586	17.408	0.527	105	37	126	16	89	42
92 [680; Glycerol-2-phosph	67 Citric acid	54 -0.340	-0.574	22.281	0.356	106	36	125	17	117	111
92 [680; Glycerol-2-phosph	4 Phosphoric acid	42 -0.366	-0.278	31.883	0.236	107	35	95	47	135	138
92 [680; Glycerol-2-phosph	36 [596; N-Acetylglutamic acid (2TMS)]	54 -0.377	-0.387	26.977	0.349	108	34	102	40	121	115
92 [680; Glycerol-2-phosph	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	43 -0.378	-0.473	20.838	0.326	109	33	112	30	105	123
92 [680; Glycerol-2-phosph	7 Threonine	54 -0.385	-0.391	28.070	0.292	110	32	103	39	124	133
92 [680; Glycerol-2-phosph	60 Glycerol-3-phosphate	54 -0.389	-0.523	20.369	0.403	111	31	118	24	103	89
92 [680; Glycerol-2-phosph	34 Aspartic acid	54 -0.391	-0.405	30.332	0.358	112	30	106	36	132	110
92 [680; Glycerol-2-phosph	37 Phenylalanine	54 -0.395	-0.555	21.535	0.366	113	29	121	21	112	105
92 [680; Glycerol-2-phosph	130 Trehalose	54 -0.398	-0.299	28.166	0.333	114	28	98	46	125	118
92 [680; Glycerol-2-phosph	75 Lysine	54 -0.410	-0.330	36.697	0.352	115	27	98	44	138	114
92 [680; Glycerol-2-phosph	48 Asparagine	54 -0.416	-0.748	15.740	0.534	116	26	132	10	80	38
92 [680; Glycerol-2-phosph	23 Homoserine	54 -0.421	-0.544	15.104	0.426	117	25	120	22	73	82
92 [680; Glycerol-2-phosph	[638; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	54 -0.423	-0.274	17.208	0.318	118	24	94	48	87	128
92 [680; Glycerol-2-phosph	8 Isoleucine	45 -0.438	-0.344	20.305	0.224	119	23	100	42	102	140
92 [680; Glycerol-2-phosph	131 [626; 5-Methylthioadenosine (3TMS)]	47 -0.443	-0.824	17.379	0.500	120	22	129	13	88	54
92 [680; Glycerol-2-phosph	98 [897; Ribose-5-phosphate methoxymine (5TMS)]	40 -0.459	-0.570	19.819	0.332	121	21	124	18	100	119
92 [680; Glycerol-2-phosph	33 Methionine	54 -0.461	-0.455	14.930	0.361	122	20	110	32	72	108
92 [680; Glycerol-2-phosph	2 Serine	52 -0.468	-0.395	20.953	0.300	123	19	104	38	107	131
92 [680; Glycerol-2-phosph	31 [622; Parabanic acid (2TMS)]	54 -0.480	-0.474	13.522	0.376	124	18	113	29	63	101
92 [680; Glycerol-2-phosph	69 Arginine	50 -0.486	-0.629	21.494	0.449	125	17	130	12	111	74
92 [680; Glycerol-2-phosph	66 Glycine	54 -0.488	-0.415	10.682	0.353	126	16	108	34	41	112
92 [680; Glycerol-2-phosph	30 [815; Ethyl-3(2H)-thiophenone]	54 -0.494	-0.481	28.201	0.314	127	15	115	27	128	129
92 [680; Glycerol-2-phosph	82 Lysine	29 -0.498	-0.818	17.972	0.476	128	14	137	5	93	63
92 [680; Glycerol-2-phosph	[826; beta-[(5-methyl-2-thienyl)methylenamino-benzeneacetic acid methyl ester]										
92 [680; Glycerol-2-phosph	77 Ornithine; Arginine	52 -0.501	-0.616	27.778	0.331	129	13	128	14	123	120
92 [680; Glycerol-2-phosph	59 Leucine	54 -0.502	-0.510	37.435	0.348	130	12	117	25	139	116
92 [680; Glycerol-2-phosph	5 Leucine	35 -0.503	-0.477	13.489	0.227	131	11	114	28	61	139
92 [680; Glycerol-2-phosph	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	34 -0.508	-0.614	18.972	0.276	132	10	127	15	95	135
92 [680; Glycerol-2-phosph	9 Proline	53 -0.512	-0.442	27.449	0.303	133	9	109	33	122	130
92 [680; Glycerol-2-phosph	3 Ethanolamine	52 -0.517	-0.772	15.143	0.492	134	8	134	8	75	58
92 [680; Glycerol-2-phosph	10 Glycine	54 -0.509	-0.794	20.053	0.585	135	7	136	6	96	13
92 [680; Glycerol-2-phosph	32 [729; N,N-Dimethyllysine methyl ester]	53 -0.553	-0.563	19.113	0.415	136	6	122	20	101	84
92 [680; Glycerol-2-phosph	68 [570; Hypoxanthine (2TMS)]	11 -0.564	-0.919	12.952	0.215	137	5	140	2	57	141
92 [680; Glycerol-2-phosph	55 [812; 4-Aminobutyric acid (2TBS)]	33 -0.572	-0.942	21.375	0.411	138	4	141	1	110	85
92 [680; Glycerol-2-phosph	42 Glutamic acid	50 -0.585	-0.587	29.647	0.324	139	3	123	19	128	124
92 [680; Glycerol-2-phosph											
20 [616; 2-(3'-4-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]		21 -0.600	-0.902	15.707	0.330	140	2	138	4	79	122

18067	92 [607; Putrescine (4TMS)	81 Tyrosine	54 -0.607	-0.792	30,790	0.561	141	1	135	7	133	24 duplicate
8779	93 [607; Putrescine (4TMS)	105 [705; 2-Ketoglucuronic acid (5TMS)]	46 0.666	0.771	17,058	0.414	141	1	141	1	141	65 original
8771	93 [607; Putrescine (4TMS)	97 [756; beta-D-Methylglucopyranoside (4TMS)]	50 0.549	0.615	27,369	0.449	2	140	6	136	100	29 original
18242	93 [607; Putrescine (4TMS)	84 Mannitol	58 0.526	0.680	40,087	0.470	3	139	3	139	122	17 duplicate
12505	93 [607; Putrescine (4TMS)	20 [619; 2-(3',4'-Bishydroxyphenyl)-2-oxethylamine (4TMS)]	29 0.522	0.721	7,012	0.529	4	138	2	140	1	2 duplicate
18662	93 [607; Putrescine (4TMS)	92 [680; Glycerol-2-phosphate (4TMS)]	51 0.467	0.243	15,299	0.368	5	137	37	105	52	101 duplicate
18512	93 [607; Putrescine (4TMS)	89 [775; Dopamine (4TMS)]	32 0.448	0.221	13,301	0.514	6	136	40	102	37	6 duplicate
8802	93 [607; Putrescine (4TMS)	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	44 0.436	0.536	15,465	0.323	7	135	8	134	53	135 original
8773	93 [607; Putrescine (4TMS)	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	40 0.418	0.433	8,552	0.360	8	134	10	132	5	110 original
18127	93 [607; Putrescine (4TMS)	82 Lysine	37 0.375	0.510	23,367	0.562	9	133	9	133	89	1 duplicate
18635	93 [607; Putrescine (4TMS)	63 Glutamine	48 0.348	0.099	15,276	0.419	10	132	58	84	51	57 duplicate
18352	93 [607; Putrescine (4TMS)	57 [757; 2-Desoxy-pentos-3-ylose dimethoxyamine (2TMS)]	53 0.334	0.300	21,065	0.357	11	131	29	113	84	116 duplicate
18110	93 [607; Putrescine (4TMS)	55 [612; 4-Aminobutyric acid (2TBS)]	40 0.333	0.313	10,326	0.507	12	130	26	116	16	7 duplicate
18563	93 [607; Putrescine (4TMS)	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	60 0.319	0.315	16,759	0.354	13	129	25	117	60	120 duplicate
10585	93 [607; Putrescine (4TMS)	5 Leucine	42 0.310	0.108	12,943	0.483	14	128	56	86	33	11 duplicate
10035	93 [607; Putrescine (4TMS)	1 [938; Sulfuric acid (2TMS)]	34 0.305	0.423	10,064	0.335	15	127	11	131	14	133 duplicate
15849	93 [607; Putrescine (4TMS)	52 [NA]	43 0.305	0.168	13,391	0.494	16	126	46	98	38	9 duplicate
8777	93 [607; Putrescine (4TMS)	103 [648; Ethylamine (2TMS)]	59 0.303	0.603	19,847	0.437	17	125	7	135	79	35 original
16024	93 [607; Putrescine (4TMS)	54 [NA]	51 0.293	0.381	11,028	0.362	18	124	13	129	22	109 duplicate
8801	93 [607; Putrescine (4TMS)	127 [777; Fructose-6-phosphate methoxyamine (8TMS)]	38 0.277	0.358	11,442	0.252	19	123	18	124	25	140 original
18813	93 [607; Putrescine (4TMS)	91 [768; beta-D-Methylglucopyranoside (4TMS)]	60 0.262	0.648	20,328	0.462	20	122	4	138	83	22 duplicate
8775	93 [607; Putrescine (4TMS)	101 [832; Dopamine (4TMS)]	60 0.261	0.630	16,750	0.461	21	121	5	137	59	23 original
11509	93 [607; Putrescine (4TMS)	12 Glycetic acid	59 0.244	0.371	9,085	0.394	22	120	14	128	9	76 duplicate
8803	93 [607; Putrescine (4TMS)	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	56 0.236	0.330	17,228	0.408	23	119	22	120	63	68 original
8808	93 [607; Putrescine (4TMS)	134 Isomaltose	60 0.227	0.297	34,843	0.431	24	118	30	112	118	43 original
15937	93 [607; Putrescine (4TMS)	53 Glycerol-2-phosphate	60 0.226	0.249	9,350	0.359	25	117	38	106	12	112 duplicate
8781	93 [607; Putrescine (4TMS)	107 9-(Z)-Octadecenoic acid	60 0.214	0.074	25,302	0.376	26	116	61	81	96	91 original
15394	93 [607; Putrescine (4TMS)	47 [NA]	60 0.206	0.338	16,762	0.420	27	114	21	121	61	56 duplicate
15579	93 [607; Putrescine (4TMS)	49 [877; Pyrophosphoric acid (4TMS)]	60 0.206	0.281	12,249	0.360	28	115	33	109	27	111 duplicate
13549	93 [607; Putrescine (4TMS)	29 Erythritol	60 0.202	0.383	14,320	0.395	29	112	16	128	41	75 duplicate
8783	93 [607; Putrescine (4TMS)	119 [931; myo-Inositol-2-phosphate (7TMS)]	60 0.202	0.194	17,283	0.352	30	113	44	98	65	122 original
11637	93 [607; Putrescine (4TMS)	13 Uracl	60 0.199	0.366	26,202	0.435	31	110	15	127	98	39 duplicate
16268	93 [607; Putrescine (4TMS)	56 [828; Oroic acid (3TMS)]	60 0.199	0.286	14,976	0.444	32	111	32	110	49	31 duplicate
16678	93 [607; Putrescine (4TMS)	61 [NA]	60 0.193	0.157	15,550	0.392	33	109	47	95	55	77 duplicate
12015	93 [607; Putrescine (4TMS)	16 [844; 2-Methyl-1,3-butanediol (2TMS)]	60 0.190	0.360	28,293	0.416	34	107	17	125	104	60 duplicate
16988	93 [607; Putrescine (4TMS)	65 [846; 3-Deoxyglucitol (5TMS)]	60 0.190	0.271	17,234	0.442	35	108	34	108	64	32 duplicate
18460	93 [607; Putrescine (4TMS)	88 Gluconic acid	60 0.180	0.384	21,372	0.466	36	106	12	130	85	20 duplicate
8809	93 [607; Putrescine (4TMS)	135 [902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	60 0.178	0.142	23,155	0.372	37	105	51	91	88	97 original
12979	93 [607; Putrescine (4TMS)	24 [725; 2-Ketocacanic acid (2TMS)]	60 0.176	0.321	42,497	0.439	38	104	24	118	130	34 duplicate
8769	93 [607; Putrescine (4TMS)	95 [770; 3,4,6-Trisubhydroxyphenylethanolamine (5TMS)]	46 0.171	0.224	11,026	0.348	39	103	39	103	21	125 original
14614	93 [607; Putrescine (4TMS)	39 [829; 1-Phenylethanol (1TMS)]	60 0.169	0.339	25,094	0.375	40	102	20	122	94	93 duplicate
15670	93 [607; Putrescine (4TMS)	50 [746; Ribonic acid-1,4-lactone (3TMS)]	57 0.168	0.353	8,705	0.363	41	101	19	123	6	108 duplicate
15300	93 [607; Putrescine (4TMS)	46 Arabinose	60 0.167	0.252	26,056	0.429	42	100	35	107	97	46 duplicate
12139	93 [607; Putrescine (4TMS)	17 [700; 2-methyl-1,2-propanediol (2TMS)]	60 0.159	0.323	28,010	0.405	43	99	23	119	103	71 duplicate
17210	93 [607; Putrescine (4TMS)	68 [570; Hypoxanthine (2TMS)]	19 0.158	-0.116	9,284	0.451	44	98	85	57	10	27 duplicate
15760	93 [607; Putrescine (4TMS)	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	42 0.134	-0.316	13,187	0.434	45	97	111	31	36	40 duplicate
14512	93 [607; Putrescine (4TMS)	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	60 0.118	0.308	17,756	0.391	46	96	27	115	68	76 duplicate

8774	93 [607; Putrescine (4TMS; 100 [857; Mannitol (6TMS)]	60	0.116	0.301	19.297	0.373	47	95	28	114	76	98 original
15205	93 [607; Putrescine (4TMS; 45 Homocysteine	57	0.115	0.116	11.084	0.305	48	94	54	88	23	137 duplicate
8786	93 [607; Putrescine (4TMS; 112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	59	0.109	0.105	8.256	0.379	49	93	57	85	3	89 original
11380	93 [607; Putrescine (4TMS; 11 Succinic acid	60	0.098	0.204	18.222	0.385	50	92	42	100	71	82 duplicate
8776	93 [607; Putrescine (4TMS; 102 [904; Galactose methoxyamine (5TMS)]	60	0.095	0.192	13.048	0.367	51	91	45	97	35	104 original
15109	93 [607; Putrescine (4TMS; 44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	48	0.094	0.111	18.437	0.343	52	90	55	87	72	128 duplicate
12744	93 [607; Putrescine (4TMS; 22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	49	0.094	0.295	9.019	0.374	53	89	31	111	8	94 duplicate
18353	93 [607; Putrescine (4TMS; 86 [793; D-Galactono-1,4-lactone (4TMS)]	57	0.075	0.092	31.036	0.468	54	88	59	83	110	19 duplicate
15487	93 [607; Putrescine (4TMS; 48 Asparagine	60	0.068	-0.051	19.310	0.441	55	87	77	65	77	33 duplicate
8784	93 [607; Putrescine (4TMS; 110 [715; Erythritol (4TMS)]	51	0.060	0.077	15.522	0.428	56	86	60	82	54	52 original
8800	93 [607; Putrescine (4TMS; 126 [559; Erythritol (4TMS)]	44	0.057	0.002	13.527	0.350	57	85	68	74	39	124 original
8796	93 [607; Putrescine (4TMS; 122 [844; Erythritol (4TMS)]	50	0.048	0.048	12.581	0.356	58	84	49	93	31	117 original
11764	93 [607; Putrescine (4TMS; 14 Fumaric acid	60	0.042	0.220	10.738	0.377	60	82	41	101	19	90 duplicate
15012	93 [607; Putrescine (4TMS; 43 [548; Leucine (2TMS)]	57	0.041	0.128	17.353	0.337	61	81	52	90	68	132 duplicate
16757	93 [607; Putrescine (4TMS; 62 [812; D-Xylofuranose (4TMS)]	60	0.035	0.148	25.012	0.381	62	80	48	94	92	87 duplicate
8810	93 [607; Putrescine (4TMS; 136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	16	0.033	-0.152	9.329	0.215	63	79	93	49	11	141 original
8794	93 [607; Putrescine (4TMS; 120 [945; Uridine (3TMS)]	53	0.025	-0.119	22.564	0.352	64	78	86	56	87	123 original
10987	93 [607; Putrescine (4TMS; 8 Isoleucine	51	0.024	-0.336	29.103	0.477	65	77	114	28	106	14 duplicate
8805	93 [607; Putrescine (4TMS; 131 [626; 5-Methylthiadenosine (3TMS)]	51	0.018	0.034	8.758	0.438	66	76	65	77	7	36 original
13437	93 [607; Putrescine (4TMS; 28 Malic acid	60	0.016	0.198	19.963	0.368	67	75	43	99	80	103 duplicate
13210	93 [607; Putrescine (4TMS; 26 Citramalic acid	60	0.005	0.050	27.327	0.364	68	74	63	79	99	107 duplicate
8791	93 [607; Putrescine (4TMS; 117 [724; Glycerol (3TMS)]	53	0.000	0.047	15.156	0.371	69	73	64	78	50	98 original
17282	93 [607; Putrescine (4TMS; 69 Arginine	56	-0.017	-0.287	31.785	0.470	70	72	108	34	111	16 duplicate
8795	93 [607; Putrescine (4TMS; 121 [657; Erythritol (4TMS)]	51	-0.021	-0.054	11.201	0.344	71	71	79	63	24	128 original
17822	93 [607; Putrescine (4TMS; 77 [826; beta-[[[5-methyl-2-thienyl]methyl]amino- benzeneacetic acid methyl ester]	58	-0.022	-0.337	40.316	0.423	72	70	115	27	125	55 duplicate
13987	93 [607; Putrescine (4TMS; 33 Methionine	60	-0.024	-0.141	19.518	0.355	73	69	91	51	78	118 duplicate
14715	93 [607; Putrescine (4TMS; 40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	60	-0.028	0.050	45.088	0.406	74	68	62	80	135	70 duplicate
8813	93 [607; Putrescine (4TMS; 139 [700; Ergosta-5,7-dien-3-ol]	36	-0.029	0.032	8.530	0.345	75	67	66	76	4	126 original
14094	93 [607; Putrescine (4TMS; 34 Aspartic acid	60	-0.031	-0.111	43.343	0.325	76	66	84	58	132	134 duplicate
13660	93 [607; Putrescine (4TMS; 30 [815; Ethyl-3(2H)-thiophenone]	60	-0.032	-0.227	40.504	0.358	77	65	99	43	126	115 duplicate
13095	93 [607; Putrescine (4TMS; 25 [709; 2,5-Diaminoverdactam (2TMS)]	46	-0.032	-0.340	18.021	0.366	78	64	118	24	70	105 duplicate
8785	93 [607; Putrescine (4TMS; 111 [583; Erythritol (4TMS)]	39	-0.036	-0.019	10.231	0.290	79	63	74	68	15	139 original
8815	93 [607; Putrescine (4TMS; 141 Lanosta-8,24-dien-3-beta-ol	58	-0.038	-0.058	10.352	0.412	80	62	80	62	17	66 original
8789	93 [607; Putrescine (4TMS; 115 Glucose-6-phosphate	58	-0.041	0.018	35.521	0.418	81	61	67	75	119	58 original
11250	93 [607; Putrescine (4TMS; 10 Glycine	60	-0.056	-0.224	29.791	0.428	82	60	98	44	108	47 duplicate
17137	93 [607; Putrescine (4TMS; 67 Citric acid	60	-0.058	-0.358	34.787	0.454	83	59	120	22	117	26 duplicate
17758	93 [607; Putrescine (4TMS; 76 Fructose	60	-0.060	-0.009	36.526	0.427	84	57	73	69	120	48 duplicate
17627	93 [607; Putrescine (4TMS; 74 [912; Tetradecanoic acid (1TMS)]	60	-0.060	-0.178	17.638	0.397	85	58	94	48	67	74 duplicate
18298	93 [607; Putrescine (4TMS; 85 [529; Methylcitric acid (4TMS)]	45	-0.061	-0.027	14.143	0.518	86	56	76	66	40	5 duplicate
14914	93 [607; Putrescine (4TMS; 42 Glutamic acid	56	-0.062	-0.002	40.124	0.418	87	55	131	11	123	59 duplicate
12625	93 [607; Putrescine (4TMS; 21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	58	-0.066	-0.002	27.709	0.402	88	54	71	71	102	73 duplicate
18407	93 [607; Putrescine (4TMS; 87 [945; beta-D-Glucopyranose (5TMS)]	58	-0.067	-0.024	45.699	0.406	89	53	75	67	136	69 duplicate
8811	93 [607; Putrescine (4TMS; 137 Ergosterol	60	-0.070	-0.276	25.091	0.383	90	52	105	37	93	85 original
17985	93 [607; Putrescine (4TMS; 78 Mannose	58	-0.074	-0.066	15.709	0.381	91	51	81	61	56	88 duplicate
14409	93 [607; Putrescine (4TMS; 37 Phenylalanine	60	-0.076	-0.372	33.911	0.446	92	50	121	21	118	30 duplicate
16517	93 [607; Putrescine (4TMS; 59 Ornithine; Arginine	60	-0.078	-0.281	51.421	0.404	93	49	106	36	139	72 duplicate
17492	93 [607; Putrescine (4TMS; 72 [919; D-Xylopyranose (4TMS)]	59	-0.080	-0.145	14.590	0.345	94	48	92	50	44	127 duplicate
8814	93 [607; Putrescine (4TMS; 140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	47	-0.086	-0.008	7.279	0.430	95	47	72	70	2	44 original
8780	93 [607; Putrescine (4TMS; 108 [733; Threitol (4TMS)]	58	-0.088	0.000	20.034	0.458	96	46	69	73	81	25 original
14200	93 [607; Putrescine (4TMS; 35 Pyroglutamic acid	60	-0.092	-0.001	51.855	0.423	97	45	70	72	140	54 duplicate



10312	93 [607; Putrescine (4TMS); 3 Ethanolamine	58 -0.099	-0.288	13,006	0.436	88	44	109	33	34	38uplicate
8782	93 [607; Putrescine (4TMS); 108 Octadecanoic acid	60 -0.099	-0.330	14,348	0.388	99	43	113	29	42	81 original
8806	93 [607; Putrescine (4TMS); 132 [895; Isomaltose methoxyamine (8TMS)]	41 -0.115	-0.237	12,093	0.292	100	42	38	104	28	138 original
8768	93 [607; Putrescine (4TMS); 94 Hexadecanoic acid	60 -0.115	-0.239	33,012	0.371	101	41	100	42	114	99 original
18068	93 [607; Putrescine (4TMS); 81 Tyrosine	60 -0.118	-0.382	44,836	0.520	102	40	122	20	134	3uplicate
12862	93 [607; Putrescine (4TMS); 23 Homoserine	60 -0.120	-0.285	20,042	0.375	103	39	107	35	82	92uplicate
8783	93 [607; Putrescine (4TMS); 109 Octadecanoic acid	60 -0.121	-0.259	33,821	0.353	104	38	102	40	115	121 original
17560	93 [607; Putrescine (4TMS); 73 [708; Glucose methoxyamine (5TMS)] 124 [734; 1-Monooleryglycerol (2TMS); 1-	53 -0.132	-0.136	15,988	0.414	105	37	90	52	57	64uplicate
8798	93 [607; Putrescine (4TMS); Monohexadecenoylglycerol (1TMS)]	55 -0.137	-0.187	12,887	0.338	106	36	95	47	32	131 original
13770	93 [607; Putrescine (4TMS); 31 [822; Parabenic acid (2TMS)]	60 -0.153	-0.337	0.368;	107	35	116	28	29	102uplicate	
17353	93 [607; Putrescine (4TMS); 70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	53 -0.154	-0.053	28,727	0.358	108	34	78	64	105	114uplicate
16598	93 [607; Putrescine (4TMS); 60 Glycerol-3-phosphate	60 -0.157	-0.406	32,729	0.464	109	33	126	16	113	21uplicate
8780	93 [607; Putrescine (4TMS); 116 [882; Pseudouridine (5TMS)]	29 -0.158	0.147	10,760	0.518	110	32	50	92	20	4 original
12282	93 [607; Putrescine (4TMS); 18 [590; 1-Acetyl-2-thiohydantoin]	60 -0.163	-0.253	18,849	0.355	111	31	101	41	74	119uplicate
8770	93 [607; Putrescine (4TMS); 96 myo-Inositol	47 -0.164	-0.125	10,054	0.314	112	30	87	55	13	138uplicate
10720	93 [607; Putrescine (4TMS); 6 Glycerol	60 -0.167	-0.110	52,317	0.390	113	29	83	59	141	79uplicate
18008	93 [607; Putrescine (4TMS); 80 [772; D-Glucose (5TMS)]	58 -0.175	-0.067	40,823	0.385	114	28	82	60	128	84uplicate
8719	93 [607; Putrescine (4TMS); 125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	60 -0.195	-0.134	43,056	0.385	115	27	88	54	131	83 original
11119	93 [607; Putrescine (4TMS); 9 Proline	60 -0.199	-0.420	38,531	0.415	116	26	128	14	121	63uplicate
13324	93 [607; Putrescine (4TMS); 27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	49 -0.199	-0.265	16,159	0.426	117	25	103	39	58	50uplicate
17423	93 [607; Putrescine (4TMS); 71 [731; Erythrose (3TMS)]	60 -0.209	-0.432	23,371	0.408	118	24	129	13	90	67uplicate
10854	93 [607; Putrescine (4TMS); 7 Threonine	60 -0.225	-0.437	41,152	0.382	119	23	130	12	129	86uplicate
8787	93 [607; Putrescine (4TMS); 113 Galactose-6-phosphate	58 -0.246	-0.135	14,615	0.433	120	22	89	53	45	42 original
13879	93 [607; Putrescine (4TMS); 32 [729; N,N-Dimethyllysine methyl ester]	59 -0.252	-0.479	19,016	0.429	121	21	133	9	75	45uplicate
8807	93 [607; Putrescine (4TMS); 133 [855; Squalene]	60 -0.258	-0.404	18,490	0.358	122	20	125	17	73	113 original
8792	93 [607; Putrescine (4TMS); 118 [928; Glucopyranose-6-phosphate (6TMS)]	55 -0.262	-0.223	14,788	0.365	123	19	97	45	48	106 original
16912	93 [607; Putrescine (4TMS); 64 [789; Tyramine (3TMS)]	59 -0.297	-0.267	14,691	0.342	124	18	104	38	47	130uplicate
8778	93 [607; Putrescine (4TMS); 104 [795; Erythritol (4TMS)]	59 -0.314	-0.410	18,004	0.468	125	17	127	15	69	18 original
8772	93 [607; Putrescine (4TMS); 98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	44 -0.315	-0.483	14,353	0.416	126	16	134	8	43	81 original
10174	93 [607; Putrescine (4TMS); 2 Serine	58 -0.318	-0.484	29,785	0.426	127	15	135	7	107	51uplicate
8788	93 [607; Putrescine (4TMS); 114 Fructose-6-phosphate	50 -0.319	-0.209	12,343	0.427	128	14	96	46	28	49 original
11890	93 [607; Putrescine (4TMS); 15 Alanine	60 -0.325	-0.339	30,019	0.479	129	13	117	25	109	13uplicate
14815	93 [607; Putrescine (4TMS); 41 [639; Proline (2TMS)]	60 -0.329	-0.352	25,186	0.368	130	12	119	23	95	100uplicate
12394	93 [607; Putrescine (4TMS); 19 Alanine (BP) (3TMS)	60 -0.331	-0.320	23,480	0.436	131	11	112	30	91	37uplicate
17063	93 [607; Putrescine (4TMS); 66 Glyceric acid-3-phosphate	60 -0.339	-0.617	14,668	0.451	132	10	140	2	46	28uplicate
8812	93 [607; Putrescine (4TMS); 138 [674; Ergosterol (1TMS)]	44 -0.353	-0.465	10,518	0.461	133	9	132	10	18	24 original
18185	93 [607; Putrescine (4TMS); 83 Sorbitol	54 -0.371	-0.396	32,175	0.501	134	8	123	19	112	8uplicate
8804	93 [607; Putrescine (4TMS); 130 Trehalose	59 -0.383	-0.523	40,576	0.389	135	7	138	4	127	80 original
10449	93 [607; Putrescine (4TMS); 4 Phosphoric acid	48 -0.385	-0.597	44,195	0.482	136	-6	139	3	133	12uplicate
8797	93 [607; Putrescine (4TMS); 123 [945; Galactofuranose-6-phosphate (7TMS)]	60 -0.388	-0.397	22,338	0.425	137	5	124	18	86	53 original
17947	93 [607; Putrescine (4TMS); 79 Glucose	60 -0.389	-0.304	46,102	0.487	138	4	110	32	137	10uplicate
14305	93 [607; Putrescine (4TMS); 38 [596; N-Acetylglutamic acid (2TMS)]	60 -0.406	-0.692	40,162	0.474	139	3	141	1	124	15uplicate
17693	93 [607; Putrescine (4TMS); 75 Lysine	60 -0.473	-0.511	50,431	0.416	140	2	137	5	138	62uplicate
16435	93 [607; Putrescine (4TMS); 58 [636; 4R-Acetamido-2,3-(2Z)-epoxy-4-(E)-hydroxycyclohexane	60 -0.507	-0.500	27,704	0.433	141	1	136	6	101	41uplicate
8830	94 Hexadecanoic acid	64 0.850	0.978	5,159	0.687	1	141	1	141	1	1 original
8837	94 Hexadecanoic acid	30 0.720	0.767	19,671	0.435	2	140	6	138	70	86 original
8859	94 Hexadecanoic acid	46 0.683	0.882	31,071	0.585	3	139	2	140	125	9 original
8858	94 Hexadecanoic acid	64 0.878	0.878	11,688	0.547	4	138	10	132	17	15 original
8892	94 Hexadecanoic acid	51 0.688	0.758	28,190	0.603	5	137	7	135	121	3 original

8847	94 Hexadecanoic acid	126 [559; Erythritol (4TMS)]	45	0.572	0.864	18.669	0.598	6	136	4	138	61	5 original
8861	94 Hexadecanoic acid	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	48	0.568	0.866	31.698	0.540	7	135	8	134	126	18 original
18299	94 Hexadecanoic acid	85 [529; Methylcitric acid (4TMS)]	49	0.562	0.834	18.513	0.531	8	134	5	137	60	25 duplicate
17628	94 Hexadecanoic acid	74 [912; Tetradecanoic acid (1TMS)]	64	0.520	0.873	20.535	0.589	9	133	3	139	76	7 duplicate
8845	94 Hexadecanoic acid	124 [734; 1-Monooctylethylglycerol (2TMS); 1-Monohexadecanoylethylglycerol (1TMS)]	59	0.490	0.511	39.777	0.458	10	132	23	119	140	71 original
8828	94 Hexadecanoic acid	107 [9-(Z)-Octadecanoic acid]	64	0.485	0.355	10.246	0.585	11	131	45	97	11	10 original
8854	94 Hexadecanoic acid	133 [855; Squalene]	64	0.487	0.682	17.865	0.494	12	130	9	133	56	45 original
17424	94 Hexadecanoic acid	71 [731; Erythrose (3TMS)]	64	0.423	0.613	11.611	0.484	13	129	15	127	15	47 duplicate
8840	94 Hexadecanoic acid	119 [931; myo-Inositol-2-phosphate (7TMS)]	64	0.420	0.494	17.612	0.539	14	128	29	113	54	19 original
15110	94 Hexadecanoic acid	44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	0.419	0.675	15.445	0.547	15	127	11	131	35	16 duplicate
8832	94 Hexadecanoic acid	111 [583; Erythritol (4TMS)]	42	0.394	0.555	34.424	0.426	16	126	19	123	134	92 original
18188	94 Hexadecanoic acid	83 Sorbitol	58	0.389	0.372	9.307	0.341	17	125	43	99	7	135 duplicate
8843	94 Hexadecanoic acid	122 [644; Erythritol (4TMS)]	52	0.380	0.647	27.911	0.550	18	124	13	129	115	14 original
8853	94 Hexadecanoic acid	132 [895; Isomaltose methoxyamine (8TMS)]	42	0.370	0.457	26.981	0.426	19	123	36	108	112	91 original
8823	94 Hexadecanoic acid	102 [904; Galactose methoxyamine (5TMS)]	64	0.344	0.497	22.082	0.407	20	122	27	115	88	103 original
16599	94 Hexadecanoic acid	60 Glycerol-3-phosphate	64	0.342	0.470	7.570	0.476	21	121	33	109	2	54 duplicate
8831	94 Hexadecanoic acid	110 [716; Erythritol (4TMS)]	54	0.335	0.603	22.703	0.599	22	120	16	126	89	4 original
8856	94 Hexadecanoic acid	135 [902; Melibiose (6TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	0.323	0.594	11.681	0.450	23	119	17	125	16	77 original
18564	94 Hexadecanoic acid	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	64	0.305	0.199	17.982	0.514	24	118	75	67	57	35 duplicate
8821	94 Hexadecanoic acid	100 [857; Mannitol (6TMS)]	64	0.303	0.481	15.110	0.412	25	117	31	111	33	98 original
8833	94 Hexadecanoic acid	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.300	0.523	33.254	0.455	26	116	21	121	132	75 original
8842	94 Hexadecanoic acid	121 [857; Erythritol (4TMS)]	55	0.279	0.646	28.172	0.527	27	115	14	128	118	28 original
8838	94 Hexadecanoic acid	117 [724; Glycerol (3TMS)]	56	0.277	0.662	19.964	0.527	28	114	12	130	73	30 original
12506	94 Hexadecanoic acid	20 [619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	0.260	-0.369	26.007	0.613	29	113	127	15	108	2 duplicate
17138	94 Hexadecanoic acid	67 Citric acid	64	0.251	0.355	8.763	0.401	30	112	44	98	4	110 duplicate
8835	94 Hexadecanoic acid	114 Fructose-6-phosphate	53	0.247	0.499	22.964	0.523	31	111	26	116	93	31 original
14716	94 Hexadecanoic acid	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.244	0.571	16.442	0.532	32	110	18	124	41	24 duplicate
8829	94 Hexadecanoic acid	108 Octadecenoic acid	64	0.240	0.189	22.744	0.435	33	109	78	64	90	87 original
8836	94 Hexadecanoic acid	115 Glucose-6-phosphate	62	0.231	0.378	9.759	0.503	34	108	41	101	8	37 original
12263	94 Hexadecanoic acid	18 [590; 1-Acetyl-2-thiohydantoin]	64	0.225	0.529	16.363	0.451	35	107	20	122	40	76 duplicate
8860	94 Hexadecanoic acid	139 [700; Ergosta-5,7-dien-3-ol]	38	0.218	0.314	33.462	0.437	36	106	50	92	133	85 original
13211	94 Hexadecanoic acid	26 Citramalic acid	64	0.212	0.503	8.836	0.411	37	105	24	118	5	99 duplicate
13438	94 Hexadecanoic acid	28 Malic acid	64	0.208	0.489	14.520	0.445	38	104	30	112	30	80 duplicate
12745	94 Hexadecanoic acid	22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.184	0.458	26.092	0.463	39	103	35	107	109	68 duplicate
17759	94 Hexadecanoic acid	76 Fructose	64	0.181	0.343	12.288	0.499	40	102	47	95	21	42 duplicate
8848	94 Hexadecanoic acid	127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.179	0.291	17.245	0.344	41	101	53	89	50	133 original
8827	94 Hexadecanoic acid	106 [733; Threitol (4TMS)]	62	0.179	0.494	17.470	0.597	42	100	28	114	53	6 original
14410	94 Hexadecanoic acid	37 Phenylalanine	64	0.177	0.244	8.652	0.406	43	99	63	79	3	106 duplicate
17665	94 Hexadecanoic acid	14 Fumaric acid	64	0.173	0.419	25.264	0.407	44	98	40	102	105	105 duplicate
14201	94 Hexadecanoic acid	35 Pyroglutamic acid	64	0.171	0.305	22.947	0.473	46	96	52	90	91	58 duplicate
8834	94 Hexadecanoic acid	113 Galactose-6-phosphate	62	0.169	0.351	23.228	0.536	47	95	46	96	98	22 original
12385	94 Hexadecanoic acid	19 Alanine (BP) (3TMS)	64	0.166	0.478	12.986	0.544	48	94	32	110	24	17 duplicate
14816	94 Hexadecanoic acid	41 [639; Proline (2TMS)]	64	0.161	0.522	10.637	0.533	49	93	22	120	12	23 duplicate
11510	94 Hexadecanoic acid	12 Glycine acid	63	0.151	0.317	27.410	0.396	50	92	49	93	114	113 duplicate
8849	94 Hexadecanoic acid	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.147	0.207	15.774	0.388	51	91	73	69	37	115 original
8825	94 Hexadecanoic acid	104 [786; Erythritol (4TMS)]	63	0.146	0.461	19.251	0.528	52	90	34	108	67	27 original
14306	94 Hexadecanoic acid	36 [596; N-Acetylglutamic acid (2TMS)]	64	0.129	0.271	12.281	0.387	53	89	57	85	20	117 duplicate
10313	94 Hexadecanoic acid	3 Ethanolamine	62	0.128	0.099	26.296	0.482	54	88	89	53	110	50 duplicate

8817	94 Hexadecanoic acid	96 myo-Inositol	49	0.124	0.269	35,454	0.323	55	87	58	84	138	139 original
8844	94 Hexadecanoic acid	123 [945; Galactofuranose-6-phosphate (7TMS)]	64	0.118	0.448	13,231	0.536	56	86	37	105	26	21 original
10855	94 Hexadecanoic acid	7 Threonine	64	0.117	0.281	13,007	0.365	57	85	54	88	25	127 duplicate
12626	94 Hexadecanoic acid	21 [878; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	0.114	0.377	9,036	0.413	58	84	42	100	6	86 duplicate
8841	94 Hexadecanoic acid	120 [945; Uridine (3TMS)]	54	0.114	0.073	12,444	0.444	59	83	100	42	22	81 original
17886	94 Hexadecanoic acid	78 Mannose	62	0.114	0.421	24,370	0.515	60	82	39	103	101	34 duplicate
8816	94 Hexadecanoic acid	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	0.112	-0.042	30,750	0.494	61	81	105	37	124	44 original
8857	94 Hexadecanoic acid	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.103	0.428	14,319	0.354	82	80	38	104	29	132 original
17561	94 Hexadecanoic acid	73 [708; Glucose methoxamine (5TMS)]	57	0.100	0.499	22,963	0.513	63	79	25	117	92	36 duplicate
8851	94 Hexadecanoic acid	130 Trehalose	63	0.100	0.110	13,284	0.382	64	78	87	55	27	129 original
18069	94 Hexadecanoic acid	81 Tyrosine	64	0.095	0.107	18,081	0.583	65	77	88	54	58	11 duplicate
14915	94 Hexadecanoic acid	42 Glutamic acid	60	0.080	-0.004	19,089	0.335	66	76	102	40	65	137 duplicate
15850	94 Hexadecanoic acid	52 [NA]	46	0.087	-0.105	30,702	0.501	67	75	109	33	123	39 duplicate
17823	94 Hexadecanoic acid	[826; beta-[[[5-methyl-2-thienyl)methyl]amino-77 benzeneacetic acid methyl ester]	62	0.057	0.084	16,747	0.375	68	74	93	49	45	121 duplicate
17354	94 Hexadecanoic acid	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	0.051	0.213	9,876	0.410	69	73	71	71	9	100 duplicate
18663	94 Hexadecanoic acid	92 [680; Glycerol-2-phosphate (4TMS)]	54	0.048	0.055	20,954	0.408	70	72	96	46	78	102 duplicate
11381	94 Hexadecanoic acid	11 Succinic acid	64	0.048	0.257	16,792	0.399	71	71	60	82	46	111 duplicate
18758	94 Hexadecanoic acid	62 [812; D-Xylofuranose (4TMS)]	64	0.037	0.234	10,926	0.460	72	70	66	78	13	69 duplicate
14513	94 Hexadecanoic acid	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.033	0.341	17,083	0.477	73	69	48	94	49	53 duplicate
18354	94 Hexadecanoic acid	88 [793; D-Galactono-1,4-lactone (4TMS)]	61	0.031	0.275	19,881	0.517	74	68	55	87	71	33 duplicate
8846	94 Hexadecanoic acid	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	0.025	0.128	16,814	0.418	75	67	84	58	47	93 original
16025	94 Hexadecanoic acid	54 [NA]	55	0.009	0.122	26,578	0.403	76	68	85	57	111	107 duplicate
15871	94 Hexadecanoic acid	50 [746; Ribonic acid-1,4-lactone (3TMS)]	61	0.009	0.236	34,848	0.455	77	65	64	78	135	74 duplicate
8826	94 Hexadecanoic acid	105 [705; 2-Keilgluconic acid (5TMS)]	48	0.007	0.022	17,793	0.477	78	64	99	43	55	52 original
16438	94 Hexadecanoic acid	[638; 4R-Acetamido-2,3-(2-epoxy-4-(E)-hydroxycyclohexane 58 (1TMS)]	64	0.004	0.181	11,849	0.362	79	63	79	63	18	130 duplicate
17694	94 Hexadecanoic acid	75 Lysine	64	-0.007	0.215	21,581	0.365	80	62	70	72	83	128 duplicate
16518	94 Hexadecanoic acid	59 Ornithine; Arginine	64	-0.013	0.008	23,224	0.338	81	61	101	41	95	136 duplicate
13550	94 Hexadecanoic acid	29 Erythritol	64	-0.015	0.220	20,486	0.472	82	60	69	73	75	59 duplicate
18353	94 Hexadecanoic acid	57 [757; 2-Desoxy-pentao-3-yose dimethoxyamine (2TMS)]	55	-0.018	0.245	18,814	0.470	83	59	62	80	84	60 duplicate
18461	94 Hexadecanoic acid	88 Gluconic acid	64	-0.019	0.210	16,612	0.523	84	56	72	70	44	32 duplicate
10721	94 Hexadecanoic acid	6	64	-0.025	0.079	23,747	0.527	85	57	94	48	99	29 duplicate
14615	94 Hexadecanoic acid	39 [829; 1-Phenylethanol (1TMS)]	63	-0.027	0.313	15,650	0.466	86	56	51	91	36	84 duplicate
15761	94 Hexadecanoic acid	51 [498; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.027	-0.277	33,217	0.415	87	55	121	21	131	84 duplicate
15938	94 Hexadecanoic acid	53 Glycerol-2-phosphate	64	-0.031	-0.339	27,933	0.464	88	54	125	17	116	65 duplicate
11251	94 Hexadecanoic acid	10 Glycine	64	-0.033	-0.272	13,484	0.476	89	53	120	22	28	55 duplicate
11638	94 Hexadecanoic acid	13 Uracil	64	-0.038	0.222	12,526	0.536	90	52	68	74	23	20 duplicate
8850	94 Hexadecanoic acid	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	59	-0.051	0.249	21,611	0.496	91	51	61	81	84	43 original
8852	94 Hexadecanoic acid	131 [826; 5-Methylthiadenosine (3TMS)]	55	-0.052	-0.557	31,768	0.588	92	50	137	5	127	8 original
10269	94 Hexadecanoic acid	56 [829; Orotic acid (3TMS)]	64	-0.053	0.196	24,942	0.483	93	49	77	65	104	48 duplicate
8855	94 Hexadecanoic acid	134 Isomaltose	64	-0.060	0.235	15,084	0.489	94	48	65	77	32	41 original
16889	94 Hexadecanoic acid	65 [646; 3-Deoxyglucitol (5TMS)]	63	-0.063	0.263	25,312	0.487	95	47	59	83	106	46 duplicate
8839	94 Hexadecanoic acid	118 [928; Glucopyranose-6-phosphate (6TMS)]	58	-0.064	0.030	23,057	0.414	96	46	97	45	94	95 original
12980	94 Hexadecanoic acid	24 [725; 2-Keilgluconic acid (2TMS)]	64	-0.065	0.224	15,417	0.529	97	45	67	75	34	26 duplicate
13661	94 Hexadecanoic acid	30 [815; Ethyl-3-(2H)-thiophenone]	64	-0.068	-0.096	16,552	0.380	98	44	108	34	43	120 duplicate
15301	94 Hexadecanoic acid	46 Arabinose	64	-0.068	0.189	18,712	0.483	99	43	76	66	62	49 duplicate
16679	94 Hexadecanoic acid	61 [NA]	64	-0.072	-0.184	20,108	0.380	100	42	111	31	74	119 duplicate
17211	94 Hexadecanoic acid	68 [570; Hypoxanthine (2TMS)]	20	-0.074	-0.461	23,448	0.433	101	41	132	10	97	88 duplicate

12016	94 Hexadecanoic acid	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	64 -0.079	0.204	10.213	0.571	102	40	74	68	10	12 duplicate
17948	94 Hexadecanoic acid	79 Glucose	64 -0.082	0.117	18.129	0.456	103	39	86	56	59	73 duplicate
17064	94 Hexadecanoic acid	66 Glycine acid-3-phosphate	64 -0.086	0.085	22.434	0.439	104	38	82	50	87	84 duplicate
18408	94 Hexadecanoic acid	87 [945; beta-D-Glucopyranose (5TMS)]	62 -0.087	0.092	19.898	0.401	105	37	80	52	72	108 duplicate
16111	94 Hexadecanoic acid	55 [612; 4-Aminobutyric acid (2TBS)]	43 -0.087	-0.237	35.811	0.502	106	36	117	25	137	38 duplicate
15488	94 Hexadecanoic acid	48 Asparagine	64 -0.090	-0.309	22.554	0.459	107	35	123	19	88	70 duplicate
12140	94 Hexadecanoic acid	17 [700; 2-methyl-1,2-propanediol (2TMS)]	64 -0.092	0.149	11.535	0.448	108	34	83	59	14	79 duplicate
13980	94 Hexadecanoic acid	32 [729; N,N-Dimethyllysine methyl ester]	63 -0.099	-0.078	29.724	0.467	109	33	107	35	122	63 duplicate
18243	94 Hexadecanoic acid	84 Mannitol	62 -0.103	-0.358	19.623	0.392	110	32	126	16	69	114 duplicate
14095	94 Hexadecanoic acid	34 Aspartic acid	64 -0.107	-0.187	17.398	0.361	111	31	112	30	52	131 duplicate
17283	94 Hexadecanoic acid	69 Arginine	60 -0.110	-0.294	16.027	0.442	112	30	122	20	38	82 duplicate
11120	94 Hexadecanoic acid	9 Proline	63 -0.115	0.169	16.903	0.331	113	28	81	61	48	138 duplicate
8824	94 Hexadecanoic acid	103 [648; Ethylamine (2TMS)]	63 -0.115	-0.032	21.124	0.385	114	29	104	38	80	118 original
18711	94 Hexadecanoic acid	93 [607; Putrescine (4TMS)]	60 -0.115	-0.239	33.012	0.371	115	27	118	24	130	123 duplicate
13771	94 Hexadecanoic acid	31 [622; Parabanic acid (2TMS)]	64 -0.118	-0.137	27.198	0.428	116	26	110	32	113	90 duplicate
16913	94 Hexadecanoic acid	64 [789; Tyramine (3TMS)]	63 -0.119	0.023	20.902	0.450	117	25	98	44	77	78 duplicate
8820	94 Hexadecanoic acid	99 [662; Ribose-5-phosphate methoxamine (BP) (5TMS)]	41 -0.122	0.087	24.216	0.462	118	24	91	51	100	67 original
13988	94 Hexadecanoic acid	33 Methionine	64 -0.122	-0.189	21.119	0.374	119	23	113	29	79	122 duplicate
10450	94 Hexadecanoic acid	4 Phosphoric acid	51 -0.131	0.072	16.503	0.294	120	22	95	47	42	141 duplicate
8818	94 Hexadecanoic acid	97 [756; beta-D-Methylglucopyranoside (4TMS)]	52 -0.140	-0.210	19.281	0.470	121	21	114	28	68	61 original
17493	94 Hexadecanoic acid	72 [919; D-Xylopyranose (4TMS)]	63 -0.151	-0.262	24.596	0.388	122	20	119	23	102	124 duplicate
10988	94 Hexadecanoic acid	8 Isoleucine	55 -0.170	0.165	14.833	0.320	123	19	82	60	31	140 duplicate
10175	94 Hexadecanoic acid	2 Serine	62 -0.175	0.179	16.246	0.343	124	18	80	62	39	134 duplicate
11891	94 Hexadecanoic acid	15 Alanine	64 -0.181	-0.059	11.900	0.461	125	17	106	36	19	68 duplicate
18009	94 Hexadecanoic acid	80 [772; D-Glucose (5TMS)]	62 -0.184	-0.005	17.318	0.410	126	16	103	39	51	101 duplicate
15580	94 Hexadecanoic acid	49 [877; Pyrophosphoric acid (4TMS)]	64 -0.188	-0.559	37.209	0.474	127	15	138	4	138	57 duplicate
16836	94 Hexadecanoic acid	63 Glutamine	52 -0.207	-0.230	28.297	0.397	128	14	115	27	120	112 duplicate
8819	94 Hexadecanoic acid	98 [697; Ribose-5-phosphate methoxamine (5TMS)]	48 -0.209	-0.430	31.820	0.433	129	13	130	12	128	89 original
8822	94 Hexadecanoic acid	101 [832; Dopamine (4TMS)]	64 -0.216	-0.230	21.513	0.365	130	12	116	26	82	128 original
18614	94 Hexadecanoic acid	91 [766; beta-D-Methylglucopyranoside (4TMS)]	64 -0.230	-0.326	25.762	0.407	131	11	124	18	107	104 duplicate
15208	94 Hexadecanoic acid	45 Homocysteine	61 -0.231	-0.495	37.923	0.413	132	10	136	6	139	97 duplicate
12663	94 Hexadecanoic acid	23 Homoserine	64 -0.244	-0.424	21.734	0.402	133	9	128	14	85	108 duplicate
16513	94 Hexadecanoic acid	89 [775; Dopamine (4TMS)]	35 -0.264	-0.452	28.037	0.501	134	8	131	11	117	40 duplicate
10586	94 Hexadecanoic acid	5 Leucine	45 -0.273	-0.708	24.748	0.470	135	7	140	2	103	62 duplicate
18128	94 Hexadecanoic acid	82 Lysine	39 -0.320	-0.713	18.755	0.557	136	6	141	1	63	13 duplicate
15395	94 Hexadecanoic acid	47 [NA]	64 -0.346	-0.480	23.559	0.478	137	5	134	8	98	51 duplicate
15013	94 Hexadecanoic acid	43 [548; Leucine (2TBS)]	60 -0.353	-0.586	19.096	0.442	138	4	139	3	68	83 duplicate
13325	94 Hexadecanoic acid	27 [615; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53 -0.366	-0.429	32.552	0.387	139	3	129	13	129	118 duplicate
10036	94 Hexadecanoic acid	1 [938; Sulfuric acid (2TMS)]	36 -0.368	-0.484	21.420	0.476	140	2	135	7	81	56 duplicate
13098	94 Hexadecanoic acid	25 [709; 2,5-Diaminovalerolactam (2TMS)]	48 -0.387	-0.465	28.243	0.456	141	1	133	9	119	72 duplicate
18514	95 [770; 3,4,6-Trishydroxy	89 [775; Dopamine (4TMS)]	26 0.848	0.881	10.368	0.616	1	141	4	138	21	4 duplicate
18129	95 [770; 3,4,6-Trishydroxy	82 Lysine	28 0.683	0.927	23.476	0.718	2	140	1	141	81	1 duplicate
16112	95 [770; 3,4,6-Trishydroxy	55 [612; 4-Aminobutyric acid (2TBS)]	35 0.657	0.837	5.377	0.592	3	139	5	137	3	6 duplicate
10587	95 [770; 3,4,6-Trishydroxy	5 Leucine	35 0.644	0.652	13.158	0.599	4	138	14	128	31	5 duplicate
17824	95 [770; 3,4,6-Trishydroxy	[626; beta-[[[5-methyl-2-phenyl]methyl]eneamino-	49 0.597	0.660	40.470	0.398	5	137	13	129	123	91 duplicate
16837	95 [770; 3,4,6-Trishydroxy	63 Glutamine	38 0.587	0.717	15.644	0.512	6	136	9	133	41	34 duplicate
11252	95 [770; 3,4,6-Trishydroxy	10 Glycine	50 0.587	0.720	31.927	0.540	7	135	7	135	112	21 duplicate
10314	95 [770; 3,4,6-Trishydroxy	3 Ethanolamine	50 0.585	0.721	11.887	0.543	8	134	6	136	25	19 duplicate
18070	95 [770; 3,4,6-Trishydroxy	81 Tyrosine	50 0.572	0.640	44.933	0.573	9	133	15	127	133	10 duplicate
15581	95 [770; 3,4,6-Trishydroxy	49 [877; Pyrophosphoric acid (4TMS)]	50 0.551	0.700	8.439	0.502	10	132	11	131	19	35 duplicate

17212	95 [770; 3,4,6-Trishydroxyp	68	[570; Hypoxanthine (2TMS)]	17	0,544	0,911	4,334	0,636	11	131	2	140	2	3 duplicate
14916	95 [770; 3,4,6-Trishydroxyp	42	Glutamic acid	48	0,532	0,493	40,520	0,418	12	130	23	119	124	79 duplicate
15851	95 [770; 3,4,6-Trishydroxyp	52	[NA]	39	0,530	0,673	8,487	0,544	13	129	12	130	17	18 duplicate
15489	95 [770; 3,4,6-Trishydroxyp	48	Asparagine	50	0,530	0,718	21,077	0,563	14	128	8	134	70	13 duplicate
17284	95 [770; 3,4,6-Trishydroxyp	69	Arginine	47	0,515	0,595	33,489	0,498	15	127	16	126	114	39 duplicate
15762	95 [770; 3,4,6-Trishydroxyp	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	38	0,491	0,540	6,225	0,513	16	126	21	121	7	33 duplicate
17139	95 [770; 3,4,6-Trishydroxyp	67	Citric acid	50	0,479	0,591	35,975	0,479	17	125	18	124	118	45 duplicate
16600	95 [770; 3,4,6-Trishydroxyp	60	Glycerol-3-phosphate	50	0,468	0,587	33,328	0,454	18	124	19	123	113	64 duplicate
13662	95 [770; 3,4,6-Trishydroxyp	30	[815; Ethyl-3(2H)-thiophenone]	50	0,466	0,412	42,111	0,416	19	123	32	110	128	82 duplicate
14411	95 [770; 3,4,6-Trishydroxyp	37	Phenylalanine	50	0,464	0,552	35,074	0,374	20	122	20	122	116	102 duplicate
15207	95 [770; 3,4,6-Trishydroxyp	45	Homocysteine	49	0,461	0,592	5,767	0,427	21	121	17	125	4	80 duplicate
16680	95 [770; 3,4,6-Trishydroxyp	61	[NA]	50	0,451	0,519	18,254	0,418	22	120	22	120	58	77 duplicate
8898	95 [770; 3,4,6-Trishydroxyp	131	[626; 5-Methylthioadenosine (3TMS)]	44	0,442	0,710	6,575	0,589	23	119	10	132	8	8 original
13989	95 [770; 3,4,6-Trishydroxyp	33	Methionine	50	0,438	0,446	21,473	0,473	24	118	27	115	74	50 duplicate
12507	95 [770; 3,4,6-Trishydroxyp	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxethylamine (4TMS)]	26	0,422	0,894	3,908	0,702	25	117	3	139	1	2 duplicate
16519	95 [770; 3,4,6-Trishydroxyp	59	Ornithine; Arginine	50	0,416	0,425	51,854	0,377	26	116	28	114	140	97 duplicate
14096	95 [770; 3,4,6-Trishydroxyp	34	Aspartic acid	50	0,358	0,371	45,079	0,471	27	115	36	106	134	54 duplicate
13881	95 [770; 3,4,6-Trishydroxyp	32	[728; N,N-Dimethyllysine methyl ester]	50	0,337	0,462	16,114	0,462	28	114	25	117	46	58 duplicate
8886	95 [770; 3,4,6-Trishydroxyp	119	[931; myo-Inositol-2-phosphate (7TMS)]	50	0,332	0,479	18,951	0,437	29	113	24	118	61	72 original
17425	95 [770; 3,4,6-Trishydroxyp	71	[731; Erythrose (3TMS)]	50	0,314	0,376	24,935	0,398	30	112	35	107	88	90 duplicate
11121	95 [770; 3,4,6-Trishydroxyp	9	Proline	49	0,281	0,425	37,922	0,328	31	111	29	113	121	126 duplicate
8891	95 [770; 3,4,6-Trishydroxyp	124	[734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	45	0,277	0,416	7,331	0,326	32	110	31	111	12	127 original
13097	95 [770; 3,4,6-Trishydroxyp	25	[709; 2,5-Diaminovalerolactam (1TMS)]	34	0,273	0,385	17,621	0,275	33	109	34	108	56	138 duplicate
13772	95 [770; 3,4,6-Trishydroxyp	31	[622; Parabanic acid (2TMS)]	50	0,262	0,392	12,968	0,354	34	108	33	109	30	114 duplicate
8875	95 [770; 3,4,6-Trishydroxyp	108	Octadecanoic acid	50	0,247	0,279	15,832	0,375	35	107	43	99	43	99 original
10989	95 [770; 3,4,6-Trishydroxyp	8	Isoleucine	42	0,233	0,300	27,755	0,380	36	106	40	102	96	96 duplicate
8874	95 [770; 3,4,6-Trishydroxyp	107	9-(Z)-Octadecenoic acid	50	0,233	0,361	27,498	0,366	37	105	37	105	94	105 original
10856	95 [770; 3,4,6-Trishydroxyp	7	Threonine	50	0,231	0,301	41,800	0,315	38	104	39	103	127	130 duplicate
8878	95 [770; 3,4,6-Trishydroxyp	111	[583; Erythritol (4TMS)]	28	0,201	0,098	6,131	0,277	39	103	55	87	6	137 original
12864	95 [770; 3,4,6-Trishydroxyp	23	Homoserine	50	0,198	0,447	21,894	0,445	40	102	26	116	77	66 duplicate
8883	95 [770; 3,4,6-Trishydroxyp	116	[882; Pseudouridine (5TMS)]	18	0,190	0,266	8,008	0,362	41	101	44	98	14	110 original
18712	95 [770; 3,4,6-Trishydroxyp	93	[607; Putrescine (4TMS)]	46	0,171	0,224	11,026	0,348	42	100	49	93	23	121 duplicate
8872	95 [770; 3,4,6-Trishydroxyp	105	[705; 2-Ketogluconic acid (5TMS)]	34	0,169	-0,025	23,413	0,457	43	99	61	81	80	59 original
18565	95 [770; 3,4,6-Trishydroxyp	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	50	0,166	0,238	19,958	0,352	44	98	47	95	66	117 duplicate
8904	95 [770; 3,4,6-Trishydroxyp	137	Ergosterol	50	0,164	0,129	24,954	0,365	45	97	53	89	89	107 original
17065	95 [770; 3,4,6-Trishydroxyp	66	Glyceric acid-3-phosphate	50	0,163	0,236	15,985	0,361	46	96	48	94	45	111 duplicate
8908	95 [770; 3,4,6-Trishydroxyp	141	Lanosta-8,24-dien-3- $\beta$ -ol	47	0,145	0,239	9,294	0,422	47	95	46	96	18	78 original
8865	95 [770; 3,4,6-Trishydroxyp	98	[697; Ribose-5-phosphate methoxamine (5TMS)]	42	0,143	0,241	7,898	0,431	48	94	45	97	13	76 original
8906	95 [770; 3,4,6-Trishydroxyp	139	[700; Ergosta-5,7-dien-3-ol]	26	0,138	0,293	6,032	0,389	49	93	41	101	5	94 original
18759	95 [770; 3,4,6-Trishydroxyp	94	Hexadecanoic acid	50	0,112	-0,042	30,750	0,494	50	92	63	79	109	40 duplicate
10176	95 [770; 3,4,6-Trishydroxyp	2	Serine	49	0,104	0,346	29,030	0,353	51	91	38	104	103	116 duplicate
14307	95 [770; 3,4,6-Trishydroxyp	36	[596; N-Acetylglutamic acid (2TMS)]	50	0,099	0,291	39,792	0,295	52	90	42	100	122	133 duplicate
8905	95 [770; 3,4,6-Trishydroxyp	138	[674; Ergosterol (1TMS)]	33	0,091	0,096	7,009	0,375	53	89	58	98	9	98 original
15014	95 [770; 3,4,6-Trishydroxyp	43	[548; Leucine (2TMS)]	44	0,090	0,202	12,127	0,543	54	88	50	92	71	20 duplicate
13326	95 [770; 3,4,6-Trishydroxyp	27	[915; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	48	0,074	0,417	13,426	0,457	55	87	30	112	32	61 duplicate
8876	95 [770; 3,4,6-Trishydroxyp	109	Octadecanoic acid	50	0,063	-0,266	28,916	0,475	56	86	73	69	102	48 original
18244	95 [770; 3,4,6-Trishydroxyp	84	Mannitol	50	0,055	-0,110	44,187	0,331	57	85	65	77	132	125 duplicate
8803	95 [770; 3,4,6-Trishydroxyp	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	7	0,048	-0,212	8,087	0,001	58	84	72	70	15	141 original
8907	95 [770; 3,4,6-Trishydroxyp	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	36	0,025	0,133	7,074	0,415	59	83	52	90	10	83 original

8895	95 [770; 3,4,6-Trisilyloxy]	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	31	0.006	-0.175	19.602	0.341	60	82	69	73	63	122 original
17695	95 [770; 3,4,6-Trisilyloxy]	75 Lysine	50	0.006	0.190	50.286	0.355	61	81	51	91	138	113 duplicate
17494	95 [770; 3,4,6-Trisilyloxy]	72 [919; D-Xylopyranose (4TMS)]	50	0.001	-0.005	17.336	0.350	62	80	60	82	54	118 duplicate
8902	95 [770; 3,4,6-Trisilyloxy]	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	50	-0.019	-0.133	25.266	0.454	63	79	67	75	90	65 original
8897	95 [770; 3,4,6-Trisilyloxy]	130 Trehalose	48	-0.022	0.029	41.678	0.288	64	78	59	83	128	135 original
8864	95 [770; 3,4,6-Trisilyloxy]	97 [756; beta-D-Methylglucopyranoside (4TMS)]	39	-0.038	-0.329	33.579	0.406	65	77	78	64	115	87 original
8894	95 [770; 3,4,6-Trisilyloxy]	127 [777; Fructose-6-phosphate methoxamine (6TMS)]	25	-0.060	-0.101	15.411	0.261	66	76	64	78	39	139 original
16437	95 [770; 3,4,6-Trisilyloxy]	[636; 4R-Accelamide-2,3-(2-epoxy-4(E)-hydroxycyclohexane (1TMS)]	50	-0.094	0.053	28.736	0.289	67	75	58	84	98	134 duplicate
15939	95 [770; 3,4,6-Trisilyloxy]	53 Glycerol-2-phosphate	50	-0.100	-0.149	12.818	0.385	68	74	68	74	29	92 duplicate
8863	95 [770; 3,4,6-Trisilyloxy]	96 myo-Inositol	36	-0.108	-0.030	7.323	0.364	69	73	62	80	11	108 original
18187	95 [770; 3,4,6-Trisilyloxy]	83 Sorbitol	44	-0.121	0.101	30.319	0.331	70	72	54	88	106	124 duplicate
10451	95 [770; 3,4,6-Trisilyloxy]	4 Phosphoric acid	38	-0.127	0.075	41.400	0.353	71	71	57	85	125	115 duplicate
18300	95 [770; 3,4,6-Trisilyloxy]	85 [529; Methylcitric acid (4TMS)]	36	-0.133	-0.277	13.438	0.483	72	70	75	67	33	43 duplicate
15398	95 [770; 3,4,6-Trisilyloxy]	47 [NA]	50	-0.149	-0.206	22.400	0.302	73	69	71	71	79	132 duplicate
8868	95 [770; 3,4,6-Trisilyloxy]	99 [682; Ribose-5-phosphate methoxamine (BP) (5TMS)]	27	-0.157	-0.419	13.801	0.308	74	68	83	59	37	131 original
8869	95 [770; 3,4,6-Trisilyloxy]	102 [904; Galactose methoxamine (5TMS)]	50	-0.162	-0.273	15.592	0.359	75	67	74	68	40	112 original
8900	95 [770; 3,4,6-Trisilyloxy]	133 [855; Squalene]	50	-0.166	-0.112	18.802	0.350	76	66	66	76	59	119 original
10037	95 [770; 3,4,6-Trisilyloxy]	1 [938; Sulfuric acid (2TMS)]	22	-0.177	-0.178	15.865	0.281	77	65	70	72	44	136 duplicate
8885	95 [770; 3,4,6-Trisilyloxy]	92 [928; Glucopyranose-6-phosphate (6TMS)]	44	-0.178	-0.344	17.112	0.365	78	64	77	65	52	106 original
18664	95 [770; 3,4,6-Trisilyloxy]	98 [680; Glycerol-2-phosphate (4TMS)]	40	-0.179	-0.544	18.740	0.323	79	63	95	47	65	128 duplicate
8893	95 [770; 3,4,6-Trisilyloxy]	126 [559; Erythritol (4TMS)]	31	-0.183	-0.400	13.687	0.462	80	62	81	61	35	57 original
8879	95 [770; 3,4,6-Trisilyloxy]	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	49	-0.190	-0.398	8.407	0.468	81	61	80	62	16	55 original
8867	95 [770; 3,4,6-Trisilyloxy]	100 [857; Mannitol (6TMS)]	50	-0.221	-0.324	21.715	0.318	82	60	76	68	76	129 original
18615	95 [770; 3,4,6-Trisilyloxy]	91 [766; beta-D-Methylglucopyranoside (4TMS)]	50	-0.246	-0.347	28.254	0.467	83	59	79	63	97	56 duplicate
11511	95 [770; 3,4,6-Trisilyloxy]	12 Glycemic acid	49	-0.248	-0.486	12.493	0.372	84	58	89	53	27	103 duplicate
15111	95 [770; 3,4,6-Trisilyloxy]	44 [910; 2-Ketogluconic acid methoxamine (4TMS)]	36	-0.260	-0.509	19.095	0.437	85	57	91	51	62	73 duplicate
8870	95 [770; 3,4,6-Trisilyloxy]	103 [648; Ethylamine (2TMS)]	49	-0.264	-0.455	26.097	0.529	86	56	86	56	92	25 original
16914	95 [770; 3,4,6-Trisilyloxy]	64 [789; Tyramine (3TMS)]	49	-0.306	-0.437	17.337	0.418	87	55	82	60	55	81 duplicate
8868	95 [770; 3,4,6-Trisilyloxy]	101 [832; Dopamine (4TMS)]	50	-0.308	-0.419	23.486	0.497	88	54	85	57	82	38 original
17629	95 [770; 3,4,6-Trisilyloxy]	74 [912; Tetradeanoic acid (1TMS)]	50	-0.309	-0.561	15.795	0.536	89	53	96	46	42	23 duplicate
8889	95 [770; 3,4,6-Trisilyloxy]	122 [644; Erythritol (4TMS)]	38	-0.314	-0.542	12.787	0.413	91	51	94	48	28	84 original
8877	95 [770; 3,4,6-Trisilyloxy]	110 [715; Erythritol (4TMS)]	40	-0.351	-0.645	16.282	0.478	92	50	115	27	49	48 original
12746	95 [770; 3,4,6-Trisilyloxy]	22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	40	-0.374	-0.540	12.200	0.374	93	49	92	50	26	101 duplicate
12264	95 [770; 3,4,6-Trisilyloxy]	18 [590; 1-Acetyl-2-thiodyantoin]	50	-0.376	-0.541	20.266	0.477	94	48	93	49	67	47 duplicate
16354	95 [770; 3,4,6-Trisilyloxy]	57 [757; 2-Desoxy-pentao-3-yose dimethoxamine (2TMS)]	41	-0.378	-0.632	24.779	0.392	95	47	108	34	87	93 duplicate
11892	95 [770; 3,4,6-Trisilyloxy]	15 Alanine	50	-0.401	-0.583	31.871	0.526	96	45	98	44	111	26 duplicate
13551	95 [770; 3,4,6-Trisilyloxy]	29 Erythritol	50	-0.401	-0.588	17.737	0.456	97	46	99	43	57	63 duplicate
8887	95 [770; 3,4,6-Trisilyloxy]	120 [945; Uridine (3TMS)]	40	-0.403	-0.478	24.417	0.374	98	44	88	54	85	100 original
8884	95 [770; 3,4,6-Trisilyloxy]	117 [724; Glycerol (3TMS)]	42	-0.403	-0.604	16.224	0.434	99	43	103	39	48	75 original
13212	95 [770; 3,4,6-Trisilyloxy]	26 Citramalic acid	50	-0.404	-0.606	28.266	0.443	100	42	104	38	105	67 duplicate
16026	95 [770; 3,4,6-Trisilyloxy]	54 [NA]	41	-0.410	-0.582	16.122	0.339	101	41	97	45	47	123 duplicate
8899	95 [770; 3,4,6-Trisilyloxy]	132 [895; Isomaltose methoxamine (8TMS)]	28	-0.413	-0.495	13.608	0.252	102	40	90	52	34	140 original
11382	95 [770; 3,4,6-Trisilyloxy]	11 Succinic acid	50	-0.417	-0.640	21.010	0.363	103	39	111	31	69	109 duplicate
17949	95 [770; 3,4,6-Trisilyloxy]	79 Glucose	50	-0.438	-0.710	46.080	0.519	104	38	126	16	137	30 duplicate
12627	95 [770; 3,4,6-Trisilyloxy]	21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	50	-0.442	-0.591	28.911	0.442	105	37	100	42	101	68 duplicate
14514	95 [770; 3,4,6-Trisilyloxy]	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	50	-0.445	-0.616	20.721	0.399	106	36	105	37	68	89 duplicate
18462	95 [770; 3,4,6-Trisilyloxy]	88 Gluconic acid	50	-0.447	-0.652	24.742	0.582	107	35	117	25	86	9 duplicate
8890	95 [770; 3,4,6-Trisilyloxy]	123 [945; Galactofuranose-6-phosphate (7TMS)]	50	-0.450	-0.618	23.898	0.498	108	34	106	36	83	37 original

8880	95 [770]: 3,4,6-Trisidroxyp	113	Galactose-6-phosphate	-0.727	16.773	0.479	109	33	129	13	51	44 original
18010	95 [770]: 3,4,6-Trisidroxyp	80	[772]: D-Glucose (5TMS)]	-0.874	42.390	0.409	110	32	119	23	129	86 duplicate
8888	95 [770]: 3,4,6-Trisidroxyp	121	[657]: Erythritol (4TMS)]	-0.878	11.558	0.472	111	31	120	22	24	52 original
16990	95 [770]: 3,4,6-Trisidroxyp	65	[646]: 3-Deoxyglucitol (5TMS)]	-0.889	21.384	0.492	112	30	124	18	73	41 duplicate
8901	95 [770]: 3,4,6-Trisidroxyp	134	isomaltose	-0.886	36.036	0.520	113	29	123	19	119	29 original
8896	95 [770]: 3,4,6-Trisidroxyp	128	[640]: Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	-0.839	21.633	0.472	114	28	110	32	75	51 original
8871	95 [770]: 3,4,6-Trisidroxyp	104	[796]: Erythritol (4TMS)]	-0.880	18.834	0.549	115	27	121	21	60	17 original
13439	95 [770]: 3,4,6-Trisidroxyp	28	Malic acid	-0.643	22.360	0.438	116	26	114	28	78	71 duplicate
14817	95 [770]: 3,4,6-Trisidroxyp	41	[639]: Proline (2TMS)]	-0.601	25.965	0.557	117	23	101	41	91	14 duplicate
11768	95 [770]: 3,4,6-Trisidroxyp	14	Fumaric acid	-0.642	13.796	0.365	118	24	112	30	36	95 duplicate
15302	95 [770]: 3,4,6-Trisidroxyp	46	Arabinose	-0.715	28.811	0.499	119	25	128	14	99	36 duplicate
16270	95 [770]: 3,4,6-Trisidroxyp	56	[828]: Orlic acid (3TMS)]	-0.708	19.658	0.523	120	22	125	17	64	28 duplicate
15872	95 [770]: 3,4,6-Trisidroxyp	55	[748]: Ribonic acid-1,4-lactone (3TMS)]	-0.604	10.908	0.437	121	21	102	40	22	74 duplicate
8882	95 [770]: 3,4,6-Trisidroxyp	115	Glucose-6-phosphate	-0.441	35.872	0.441	122	20	131	11	117	70 original
12017	95 [770]: 3,4,6-Trisidroxyp	16	[644]: 2-Methyl-1,3-butanediol (2TMS)]	-0.638	30.521	0.553	123	18	109	33	108	15 duplicate
12141	95 [770]: 3,4,6-Trisidroxyp	17	[700]: 2-methyl-1,2-propanediol (2TMS)]	-0.645	30.434	0.410	124	19	116	26	107	85 duplicate
12881	95 [770]: 3,4,6-Trisidroxyp	24	[725]: 2-Ketooctanoic acid (2TMS)]	-0.873	42.933	0.569	125	17	118	24	131	11 duplicate
17355	95 [770]: 3,4,6-Trisidroxyp	74	[693]: 2-Furan-2-hydroxyacetic acid (2TMS)]	-0.424	29.108	0.457	126	16	84	58	104	60 duplicate
14717	95 [770]: 3,4,6-Trisidroxyp	40	[680]: 2,3-Dimethylsuccinic acid (2TMS)]	-0.886	45.437	0.472	127	15	122	20	135	53 duplicate
14616	95 [770]: 3,4,6-Trisidroxyp	39	[829]: 1-Phenylethanol (1TMS)]	-0.507	27.512	0.400	128	14	107	35	95	88 duplicate
14202	95 [770]: 3,4,6-Trisidroxyp	35	Pyroglutamic acid	-0.513	51.289	0.515	129	13	136	6	139	32 duplicate
8881	95 [770]: 3,4,6-Trisidroxyp	114	Fructose-6-phosphate	-0.753	14.117	0.474	130	12	132	10	38	49 original
11639	95 [770]: 3,4,6-Trisidroxyp	13	Uracil	-0.642	28.856	0.553	131	10	113	29	100	16 duplicate
17600	95 [770]: 3,4,6-Trisidroxyp	87	Fructose	-0.527	36.285	0.525	132	11	139	3	120	27 duplicate
18409	95 [770]: 3,4,6-Trisidroxyp	87	[945]: beta-D-Glucopyranose (5TMS)]	-0.528	45.538	0.370	133	9	130	12	138	104 duplicate
16759	95 [770]: 3,4,6-Trisidroxyp	62	[812]: D-Xylofuranose (4TMS)]	-0.711	27.305	0.442	134	8	127	15	93	69 duplicate
17887	95 [770]: 3,4,6-Trisidroxyp	78	Mannose	-0.537	17.158	0.457	135	7	133	9	53	62 duplicate
17562	95 [770]: 3,4,6-Trisidroxyp	73	[708]: Glucose methoxyamine (5TMS)]	-0.541	16.463	0.539	136	6	137	5	50	22 duplicate
8873	95 [770]: 3,4,6-Trisidroxyp	106	[733]: Threitol (4TMS)]	-0.770	21.268	0.567	137	5	134	8	72	12 original
18355	95 [770]: 3,4,6-Trisidroxyp	86	[793]: D-Galactono-1,4-lactone (4TMS)]	-0.816	31.456	0.532	138	4	140	2	110	24 duplicate
10722	95 [770]: 3,4,6-Trisidroxyp	6	Glycerol	-0.777	52.206	0.516	139	3	135	7	141	31 duplicate
12386	95 [770]: 3,4,6-Trisidroxyp	19	Alanine (BP) (3TMS)]	-0.610	24.218	0.591	140	2	138	4	84	7 duplicate
8892	95 [770]: 3,4,6-Trisidroxyp	125	[892]: Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru	-0.623	42.822	0.485	141	1	141	1	130	42 original
8928	96 myo-Inositol	116	[882]: Pseudouridine (5TMS)]	0.738	12.342	0.272	1	141	1	141	30	122 original
8923	96 myo-Inositol	111	[583]: Erythritol (4TMS)]	0.605	2.285	0.370	2	140	2	140	1	14 original
8944	96 myo-Inositol	132	[695]: Isomaltose methoxyamine (8TMS)]	0.516	10.842	0.297	3	139	3	139	25	104 original
8924	96 myo-Inositol	112	[877]: beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	0.420	5.318	0.358	4	138	6	138	6	31 original
8914	96 myo-Inositol	102	[904]: Galactose methoxyamine (5TMS)]	0.279	15.422	0.339	5	137	19	123	43	46 original
8926	96 myo-Inositol	114	Fructose-6-phosphate	0.425	12.476	0.346	6	136	5	137	32	40 original
8947	96 myo-Inositol	135	[902]: Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	0.440	25.601	0.331	7	135	4	138	89	57 original
8935	96 myo-Inositol	123	[945]: Galactofuranose-6-phosphate (7TMS)]	0.297	23.836	0.345	8	134	14	128	87	43 original
8927	96 myo-Inositol	115	Glucose-6-phosphate	0.251	36.099	0.292	9	133	26	118	118	111 original
13213	96 myo-Inositol	26	Citramalic acid	0.353	29.351	0.351	10	132	9	133	101	36 duplicate
8925	96 myo-Inositol	113	Galactose-6-phosphate	0.248	14.990	0.290	11	131	27	115	42	115 original
12747	96 myo-Inositol	22	[690]: N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	0.296	9.404	0.268	12	130	15	127	15	125 duplicate
8912	96 myo-Inositol	100	[857]: Mannitol (6TMS)]	0.342	22.040	0.353	13	129	12	130	80	35 original
13440	96 myo-Inositol	28	Malic acid	0.335	22.341	0.345	14	128	16	126	83	42 duplicate
12628	96 myo-Inositol	21	[678]: N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	0.317	29.358	0.317	15	127	11	131	102	77 duplicate
11767	96 myo-Inositol	14	Fumaric acid	0.286	12.356	0.307	16	126	18	124	31	92 duplicate

14203	96 myo-Inositol	35	Pyroglutamic acid	49	0.308	0.211	51,459	0.399	17	125	49	93	139	4	uplicate
12265	96 myo-Inositol	18	[590; 1-Acetyl-2-thiohydantoin]	49	0.303	0.327	20,654	0.279	18	123	10	132	74	120	uplicate
11893	96 myo-Inositol	15	Alanine	49	0.303	0.171	29,968	0.344	19	124	60	82	106	44	uplicate
17356	96 myo-Inositol	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	46	0.295	0.261	30,686	0.298	20	122	24	118	109	102	uplicate
8937	96 myo-Inositol	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	49	0.293	0.226	41,745	0.330	21	121	31	111	126	58	original
16760	96 myo-Inositol	62	[812; D-Xylofuranose (4TMS)]	49	0.287	0.244	26,982	0.297	22	120	28	114	94	105	uplicate
8952	96 myo-Inositol	140	[892; Ergosta-7,22-dien-3-ol (1TMS)]	42	0.267	0.395	5,140	0.338	23	119	8	134	5	47	original
111363	96 myo-Inositol	11	Succinic acid	49	0.277	0.273	20,284	0.300	24	118	20	122	73	100	uplicate
111512	96 myo-Inositol	12	Glyceric acid	48	0.273	0.291	10,491	0.286	25	117	17	125	73	119	uplicate
12387	96 myo-Inositol	106	[733; Threitol (4TMS)]	47	0.271	0.221	21,913	0.369	26	116	36	106	79	20	original
14718	96 myo-Inositol	19	Alanine (BP) (3TMS)	49	0.269	0.263	24,449	0.304	27	115	32	119	88	98	uplicate
16915	96 myo-Inositol	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	49	0.267	0.223	45,856	0.335	28	114	32	110	136	53	uplicate
14818	96 myo-Inositol	64	[788; Tyramine (3TMS)]	48	0.264	0.147	16,151	0.299	29	113	66	76	50	101	uplicate
17563	96 myo-Inositol	41	[639; Proline (2TMS)]	49	0.262	0.264	26,647	0.287	30	112	22	120	93	116	uplicate
17761	96 myo-Inositol	73	[708; Glucose methoxyamine (5TMS)]	45	0.259	0.213	15,783	0.318	31	111	43	99	45	75	uplicate
16027	96 myo-Inositol	76	Fructose	49	0.257	0.222	36,581	0.346	32	110	33	109	119	39	uplicate
17630	96 myo-Inositol	54	[NA]	40	0.244	0.231	12,007	0.307	33	109	30	112	27	90	uplicate
12018	96 myo-Inositol	74	[912; Tetradecanoic acid (1TMS)]	49	0.243	0.306	18,620	0.321	34	108	13	129	62	71	uplicate
12982	96 myo-Inositol	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	49	0.231	0.219	29,928	0.320	35	107	38	104	104	72	uplicate
17426	96 myo-Inositol	24	[725; 2-Ketooctanoic acid (2TMS)]	49	0.219	0.213	42,806	0.308	36	105	44	98	131	93	uplicate
14515	96 myo-Inositol	71	[731; Erythrose (3TMS)]	49	0.219	0.211	25,801	0.431	37	106	50	92	90	1	uplicate
17888	96 myo-Inositol	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	49	0.218	0.235	20,115	0.292	38	104	29	113	71	112	uplicate
8933	96 myo-Inositol	29	Erythritol	49	0.214	0.213	16,770	0.294	39	102	47	95	55	109	uplicate
11640	96 myo-Inositol	78	Mannose	49	0.214	0.154	16,201	0.295	40	103	65	77	51	108	uplicate
18188	96 myo-Inositol	121	[657; Erythritol (4TMS)]	40	0.208	0.213	10,198	0.317	41	101	42	100	19	80	original
8932	96 myo-Inositol	13	Ureid	49	0.202	0.213	27,842	0.318	42	100	45	97	98	76	uplicate
16991	96 myo-Inositol	83	Sorbitol	46	0.202	0.033	34,014	0.373	43	99	81	61	112	13	uplicate
8929	96 myo-Inositol	120	[945; Uridine (3TMS)]	40	0.197	0.043	23,157	0.228	44	98	80	62	86	136	original
16271	96 myo-Inositol	65	[646; 3-Deoxyglucitol (5TMS)]	48	0.195	0.221	18,163	0.346	45	97	35	107	59	38	uplicate
18463	96 myo-Inositol	117	[724; Glycerol (3TMS)]	42	0.194	0.196	16,998	0.319	46	96	56	86	57	73	original
12142	96 myo-Inositol	88	Gluconic acid	49	0.194	0.222	23,125	0.312	47	93	34	108	85	86	uplicate
8946	96 myo-Inositol	17	[700; 2-methyl-1,2-propanediol (2TMS)]	49	0.194	0.207	29,453	0.304	48	94	53	89	103	96	uplicate
14617	96 myo-Inositol	56	[829; Orolic acid (3TMS)]	49	0.189	0.215	16,326	0.338	50	92	41	101	52	48	uplicate
15303	96 myo-Inositol	134	Isomaltose	49	0.180	0.219	35,171	0.310	51	91	39	103	114	89	original
8938	96 myo-Inositol	39	[829; 1-Phenylmethanol (1TMS)]	48	0.179	0.220	26,513	0.326	52	90	37	105	91	64	uplicate
8950	96 myo-Inositol	46	Arabinose	49	0.177	0.213	26,631	0.369	53	89	46	96	92	18	uplicate
18410	96 myo-Inositol	126	[559; Erythritol (4TMS)]	31	0.174	0.185	14,584	0.230	54	88	59	83	40	135	original
8951	96 myo-Inositol	138	[674; Ergosterol (1TMS)]	39	0.171	0.419	5,491	0.332	55	87	7	135	7	56	original
8922	96 myo-Inositol	118	[928; Glucopyranose-6-phosphate (5TMS)]	43	0.169	0.070	14,372	0.307	56	86	74	68	39	91	original
17650	96 myo-Inositol	87	[945; beta-D-Glucopyranose (5TMS)]	47	0.169	0.158	44,151	0.304	57	85	64	78	132	97	uplicate
18301	96 myo-Inositol	139	[700; Ergosta-5,7-dien-3-ol]	32	0.161	-0.036	3,821	0.263	58	84	93	49	2	127	original
8948	96 myo-Inositol	80	[772; D-Glucose (5TMS)]	47	0.158	0.118	39,890	0.298	59	83	70	72	122	103	uplicate
8948	96 myo-Inositol	110	[715; Erythritol (4TMS)]	39	0.155	0.160	16,493	0.259	60	82	63	73	54	128	original
8948	96 myo-Inositol	79	Glucose	49	0.151	0.123	45,210	0.324	61	81	68	74	135	68	uplicate
8948	96 myo-Inositol	85	[528; Methyldictric acid (4TMS)]	41	0.151	0.212	16,093	0.286	62	80	48	94	48	118	uplicate
8948	96 myo-Inositol	136	[748; D-Scotoheptulose-7-phosphate (7TMS)]	16	0.150	0.199	10,251	0.088	63	79	54	88	20	141	original
8941	96 myo-Inositol	129	[840; Maltose methoxyamine (6TMS); alpha-D-Glc-(1,4)-D-Glc]	44	0.144	0.196	18,600	0.368	64	78	55	87	61	22	original
15112	96 myo-Inositol	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	35	0.143	0.189	19,780	0.238	65	77	58	84	67	133	uplicate
15673	96 myo-Inositol	50	[746; Ribic acid-1,4-lactone (3TMS)]	46	0.136	0.164	5,581	0.292	66	76	62	80	8	113	uplicate
10723	96 myo-Inositol	6	Glycerol	49	0.134	0.107	51,669	0.258	67	75	72	70	140	129	uplicate



8918	96 myo-Inositol	104 [795; Erythritol (4TMS)]	48	0.133	0.008	18,795	0.326	68	74	84	58	63	65 original
8934	96 myo-Inositol	122 [644; Erythritol (4TMS)]	37	0.132	0.124	12,283	0.316	69	73	67	75	29	82 original
18356	96 myo-Inositol	86 [793; D-Galactono-1,4-lactone (4TMS)]	47	0.130	0.209	29,956	0.328	71	72	51	91	105	62 duplicate
18760	96 myo-Inositol	94 Hexadecanoic acid	49	0.124	0.268	35,454	0.323	70	71	21	121	115	69 duplicate
8915	96 myo-Inositol	103 [648; Ethylamine (2TMS)]	48	0.119	0.061	22,697	0.361	72	70	76	66	84	29 original
8921	96 myo-Inositol	109 Octadecanoic acid	49	0.109	0.251	35,975	0.295	73	69	25	117	117	107 original
16355	96 myo-Inositol	57 [757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	40	0.105	0.169	21,817	0.251	74	68	61	81	78	131 duplicate
18665	96 myo-Inositol	92 [680; Glycerol-2-phosphate (4TMS)]	39	0.099	0.122	16,114	0.247	75	67	69	73	49	132 duplicate
8945	96 myo-Inositol	133 [855; Squalene]	48	0.088	-0.034	19,870	0.316	76	66	92	50	69	81 original
8953	96 myo-Inositol	141 Lanosta-8,24-dien-3-beta-ol	48	0.087	0.088	10,288	0.330	77	65	73	69	21	59 original
8913	96 myo-Inositol	101 [832; Dopamine (4TMS)]	49	0.078	0.054	19,986	0.369	78	64	77	65	70	15 original
18616	96 myo-Inositol	91 [766; beta-D-Methylglucopyranoside (4TMS)]	49	0.077	0.029	22,252	0.428	79	63	82	60	81	2 duplicate
8949	96 myo-Inositol	137 Ergosterol	49	0.075	0.010	27,459	0.363	80	62	83	59	95	26 original
10857	96 myo-Inositol	7 Threonine	49	0.061	-0.032	42,519	0.396	81	61	91	51	130	6 duplicate
16801	96 myo-Inositol	60 Glycerol-3-phosphate	49	0.051	0.108	34,860	0.368	82	60	71	71	113	21 duplicate
8939	96 myo-Inositol	127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	27	0.048	0.207	13,948	0.313	83	59	52	90	36	84 original
10038	96 myo-Inositol	1 [938; Sulfuric acid (2TMS)]	26	0.034	0.217	10,733	0.335	84	58	40	102	24	51 duplicate
8940	96 myo-Inositol	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	31	0.024	0.062	17,899	0.221	85	57	75	67	58	138 original
14412	96 myo-Inositol	37 Phenylalanine	49	0.009	-0.005	35,823	0.363	86	56	86	56	116	27 duplicate
17213	96 myo-Inositol	68 [570; Hypoxanthine (2TMS)]	19	0.006	-0.478	5,890	0.334	87	55	141	1	9	55 duplicate
8909	96 myo-Inositol	97 [756; beta-D-Methylglucopyranoside (4TMS)]	37	-0.024	-0.011	27,641	0.265	88	54	87	55	96	128 original
15397	96 myo-Inositol	47 [NA]	49	-0.043	-0.091	18,931	0.317	89	53	99	43	64	78 duplicate
16438	96 myo-Inositol	[936; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	49	-0.054	-0.060	28,158	0.379	90	52	95	47	100	11 duplicate
17696	96 myo-Inositol	75 Lysine	49	-0.058	-0.101	51,146	0.384	91	50	100	42	138	9 duplicate
10177	96 myo-Inositol	2 Serine	49	-0.058	-0.121	30,462	0.398	92	51	104	38	108	5 duplicate
17495	96 myo-Inositol	72 [918; D-Xylopyranose (4TMS)]	49	-0.061	-0.073	15,945	0.313	93	49	96	46	48	85 duplicate
18245	96 myo-Inositol	84 Mannitol	47	-0.066	0.052	40,392	0.318	94	48	79	63	123	74 duplicate
8936	96 myo-Inositol	124 [734; 1-Monooctylethylene glycol (2TMS); 1-Monohexadecanoglycerol (1TMS)]	47	-0.068	-0.108	4,849	0.327	95	47	102	40	4	63 original
17140	96 myo-Inositol	67 Citric acid	49	-0.070	-0.038	36,781	0.410	96	46	94	48	120	3 duplicate
15652	96 myo-Inositol	52 [NA]	34	-0.073	0.053	12,162	0.381	97	45	78	64	28	10 duplicate
8920	96 myo-Inositol	108 Octadecanoic acid	49	-0.083	-0.078	15,757	0.290	98	44	98	44	44	114 original
8931	96 myo-Inositol	119 [931; myo-Inositol-2-phosphate (7TMS)]	49	-0.092	-0.001	20,883	0.390	99	43	85	57	75	8 original
10315	96 myo-Inositol	3 Ethanolamine	48	-0.094	-0.126	14,013	0.369	100	42	108	34	37	17 duplicate
10452	96 myo-Inositol	4 Phosphoric acid	42	-0.094	-0.197	44,634	0.269	101	41	125	17	133	123 duplicate
8917	96 myo-Inositol	105 [705; 2-Ketogluconic acid (5TMS)]	33	-0.098	-0.018	19,793	0.222	102	40	88	54	68	137 original
13327	96 myo-Inositol	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	42	-0.099	-0.204	14,014	0.253	103	39	127	15	38	130 duplicate
18806	96 myo-Inositol	95 [770; 3,4,6-Trisubstituted phenylethanolamine (5TMS)]	36	-0.108	-0.030	7,323	0.364	104	38	89	53	11	25 duplicate
18566	96 myo-Inositol	90 [910; 9-(Z)-Hexadecanoic acid (1TMS)]	49	-0.111	-0.078	20,175	0.347	105	37	97	45	72	37 duplicate
13882	96 myo-Inositol	32 [729; N,N-Dimethyllysine methyl ester]	49	-0.114	-0.153	16,832	0.312	106	36	114	28	56	87 duplicate
8942	96 myo-Inositol	130 Trehalose	48	-0.121	-0.136	41,746	0.357	107	35	110	32	127	33 original
17825	96 myo-Inositol	[826; beta-[(5-methyl-2-thenyl)methyl]amino-benzeneacetic acid methyl ester]	48	-0.137	-0.158	42,479	0.358	108	34	116	26	129	32 duplicate
8911	96 myo-Inositol	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	31	-0.140	-0.031	10,104	0.220	109	33	90	52	18	139 original
14308	96 myo-Inositol	36 [596; N-Acetylglutamic acid (2TMS)]	49	-0.141	-0.130	41,338	0.364	110	31	109	33	124	24 duplicate
16681	96 myo-Inositol	61 [NA]	49	-0.141	-0.146	18,430	0.294	111	32	113	29	60	110 duplicate
18071	96 myo-Inositol	81 Tyrosine	49	-0.146	-0.162	46,919	0.329	112	30	118	24	137	60 duplicate
8919	96 myo-Inositol	107 9-(Z)-Octadecanoic acid	49	-0.153	-0.105	28,123	0.328	113	29	101	41	99	61 original
13663	96 myo-Inositol	30 [815; Ethyl-3(2H)-thiophenone]	49	-0.155	-0.122	42,093	0.361	114	27	105	37	128	30 duplicate

14097	96 myo-Inositol	34 Aspartic acid	49 -0.155	-0.142	44.754	0.311	115	28	112	30	134	88 duplicate
10588	96 myo-Inositol	5 Leucine	39 -0.155	-0.116	14.813	0.194	116	26	103	39	41	140 duplicate
11122	96 myo-Inositol	9 Proline	49 -0.160	-0.178	39.793	0.377	117	25	122	20	121	28 duplicate
13773	96 myo-Inositol	31 [62; 2-Parabanic acid (2TMS)]	49 -0.162	-0.225	12.762	0.363	118	24	131	11	33	28 duplicate
15763	96 myo-Inositol	51 [49; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	36 -0.162	-0.200	7.586	0.269	119	23	128	16	12	124 duplicate
18713	96 myo-Inositol	83 [607; Putrescine (4TMS)]	47 -0.164	-0.120	10.054	0.314	120	22	107	35	17	83 duplicate
10990	96 myo-Inositol	6 Isoleucine	46 -0.175	-0.160	30.288	0.297	121	21	117	25	107	106 duplicate
17066	96 myo-Inositol	66 Glycine acid-3-phosphate	49 -0.179	-0.158	15.961	0.357	122	20	115	27	47	34 duplicate
13990	96 myo-Inositol	33 Methionine	49 -0.192	-0.140	21.444	0.324	123	19	111	31	76	67 duplicate
12865	96 myo-Inositol	23 Homoserine	49 -0.199	-0.281	21.458	0.305	124	18	134	8	77	94 duplicate
17285	96 myo-Inositol	69 Arginine	47 -0.203	-0.219	33.354	0.305	125	17	130	12	111	95 duplicate
16113	96 myo-Inositol	55 [612; 4-Aminobutyric acid (2TBS)]	36 -0.203	-0.174	9.778	0.235	126	16	121	21	16	134 duplicate
15015	96 myo-Inositol	43 [548; Leucine (2TBS)]	47 -0.227	-0.271	18.195	0.335	127	15	135	7	65	52 duplicate
11253	96 myo-Inositol	10 Glycine	49 -0.230	-0.253	32.321	0.322	128	14	133	9	110	70 duplicate
18130	96 myo-Inositol	82 Lysine	37 -0.231	-0.210	27.823	0.286	129	13	128	14	97	117 duplicate
14917	96 myo-Inositol	42 Glutamic acid	47 -0.232	-0.184	41.423	0.325	130	12	123	19	125	66 duplicate
15208	96 myo-Inositol	45 Homocysteine	46 -0.235	-0.168	5.957	0.336	131	11	119	23	10	50 duplicate
13098	96 myo-Inositol	25 [709; 2,5-Diaminovalerolactam (2TMS)]	33 -0.250	-0.122	13.230	0.369	132	10	106	38	34	19 duplicate
16520	96 myo-Inositol	59 Ornithine; Arginine	49 -0.253	-0.195	52.282	0.369	133	9	124	18	141	16 duplicate
15490	96 myo-Inositol	48 Asparagine	49 -0.262	-0.301	22.291	0.338	134	8	137	5	82	49 duplicate
8910	96 myo-Inositol	98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	38 -0.266	-0.322	8.800	0.365	135	7	139	3	14	23 original
15940	96 myo-Inositol	53 Glycerol-2-phosphate	49 -0.289	-0.173	11.144	0.395	136	6	120	22	26	7 duplicate
16838	96 myo-Inositol	63 Glutamine	41 -0.305	-0.323	19.250	0.345	137	5	140	2	66	41 duplicate
8943	96 myo-Inositol	131 [628; 5-Methylthioadenosine (3TMS)]	41 -0.315	-0.277	7.937	0.334	138	4	136	6	13	54 original
12508	96 myo-Inositol	20 [619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	26 -0.323	-0.232	10.443	0.340	139	3	132	10	22	45 duplicate
18515	96 myo-Inositol	89 [775; Dopamine (4TMS)]	31 -0.346	-0.214	16.429	0.317	140	2	129	13	53	79 duplicate
15582	96 myo-Inositol	49 [877; Pyrophosphoric acid (4TMS)]	49 -0.364	-0.316	13.427	0.300	141	1	138	4	35	99 duplicate
8959	97 [756; beta-D-Methylgluc	103 [646; Ethylamine (2TMS)]	52 0.846	0.913	9.524	0.592	1	141	1	141	2	13 original
18617	97 [756; beta-D-Methylgluc	91 [766; beta-D-Methylglucopyranoside (4TMS)]	52 0.784	0.907	9.839	0.604	2	140	3	139	5	10 duplicate
8957	97 [756; beta-D-Methylgluc	101 [832; Dopamine (4TMS)]	52 0.765	0.897	12.634	0.556	3	139	4	138	15	40 original
8961	97 [756; beta-D-Methylgluc	105 [705; 2-Ketogluconic acid (5TMS)]	48 0.754	0.911	12.201	0.585	4	138	2	140	12	19 original
18668	97 [756; beta-D-Methylgluc	92 [680; Glycerol-2-phosphate (4TMS)]	50 0.683	0.797	16.623	0.519	5	137	14	128	38	53 duplicate
8990	97 [756; beta-D-Methylgluc	134 Isomaltose	52 0.676	0.838	11.925	0.585	6	136	6	136	11	20 original
11641	97 [756; beta-D-Methylgluc	13 Uracil	52 0.638	0.819	10.493	0.562	7	135	8	134	6	33 duplicate
8955	97 [756; beta-D-Methylgluc	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	39 0.625	0.792	21.529	0.591	8	134	16	126	74	15 original
16992	97 [756; beta-D-Methylgluc	65 [646; 3-Deoxyglucitol (5TMS)]	52 0.621	0.800	15.441	0.568	9	133	13	129	23	29 duplicate
15304	97 [756; beta-D-Methylgluc	46 Arabinose	52 0.614	0.843	8.703	0.571	10	132	5	137	1	28 duplicate
16272	97 [756; beta-D-Methylgluc	56 [929; Orolic acid (3TMS)]	52 0.612	0.837	16.537	0.577	11	131	7	135	37	23 duplicate
8985	97 [756; beta-D-Methylgluc	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	52 0.611	0.817	14.543	0.557	12	130	9	133	20	39 original
16356	97 [756; beta-D-Methylgluc	57 [757; 2-Desoxy-pentose-3-ylose dimethoxyamine (2TMS)]	50 0.600	0.817	11.373	0.591	13	129	10	132	8	17 duplicate
18464	97 [756; beta-D-Methylgluc	88 Gluconic acid	52 0.585	0.753	12.348	0.606	14	128	21	121	13	9 duplicate
12019	97 [756; beta-D-Methylgluc	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	52 0.581	0.783	11.900	0.576	15	127	15	127	10	25 duplicate
12983	97 [756; beta-D-Methylgluc	24 [725; 2-Ketooctanoic acid (2TMS)]	52 0.564	0.803	18.849	0.591	16	126	12	130	55	16 duplicate
18714	97 [756; beta-D-Methylgluc	93 [607; Putrescine (4TMS)]	50 0.549	0.815	27.369	0.449	17	125	32	110	111	85 duplicate
15674	97 [756; beta-D-Methylgluc	50 [746; Ribonic acid-1,4-lactone (3TMS)]	52 0.546	0.789	29.928	0.516	18	124	17	125	127	58 duplicate
12143	97 [756; beta-D-Methylgluc	17 [700; 2-methyl-1,2-propanediol (2TMS)]	52 0.537	0.765	11.749	0.562	19	123	19	123	9	34 duplicate
14618	97 [756; beta-D-Methylgluc	39 [828; 1-Phenylethanol (1TMS)]	52 0.534	0.738	10.680	0.483	20	122	24	118	7	70 duplicate
13553	97 [756; beta-D-Methylgluc	29 Erythritol	52 0.523	0.740	19.214	0.550	21	121	22	120	57	42 duplicate

8984	97 [756; beta-D-Methylgluc	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	44	0.507	0.675	14.764	0.517	22	120	27	115	21	56 original
18357	97 [756; beta-D-Methylgluc	86 [793; D-Galactono-1,4-lactone (4TMS)]	49	0.500	0.805	9.602	0.576	23	119	11	131	3	24 duplicate
16028	97 [756; beta-D-Methylgluc	54 [NA]	50	0.494	0.776	21.592	0.556	24	118	18	124	77	41 duplicate
14516	97 [756; beta-D-Methylgluc	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	52	0.448	0.696	16.220	0.508	25	117	26	116	34	81 duplicate
11384	97 [756; beta-D-Methylgluc	11 Succinic acid	52	0.439	0.660	16.845	0.511	26	116	28	114	40	59 duplicate
16761	97 [756; beta-D-Methylgluc	62 [812; D-Xylofuranose (4TMS)]	52	0.430	0.739	13.622	0.559	27	115	23	119	17	37 duplicate
10039	97 [756; beta-D-Methylgluc	1 [938; Sulfuric acid (2TMS)]	36	0.422	0.762	18.847	0.587	28	114	20	122	54	12 duplicate
12748	97 [756; beta-D-Methylgluc	2 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	46	0.414	0.655	22.466	0.497	29	113	29	113	85	69 duplicate
11513	97 [756; beta-D-Methylgluc	12 Glyceric acid	52	0.403	0.585	24.406	0.453	30	112	34	108	96	79 duplicate
15398	97 [756; beta-D-Methylgluc	47 [NA]	52	0.347	0.534	18.040	0.506	31	111	39	103	47	62 duplicate
11768	97 [756; beta-D-Methylgluc	14 Fumaric acid	52	0.336	0.627	22.774	0.440	32	110	31	111	89	92 duplicate
8983	97 [756; beta-D-Methylgluc	127 [777; Fructose-6-phosphate methoxymamine (6TMS)]	39	0.333	0.451	18.726	0.449	33	109	44	98	52	84 original
18246	97 [756; beta-D-Methylgluc	84 Mannitol	50	0.304	0.708	16.145	0.607	34	108	25	117	31	8 duplicate
17357	97 [756; beta-D-Methylgluc	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	45	0.295	0.391	14.051	0.565	35	107	53	89	18	30 duplicate
18411	97 [756; beta-D-Methylgluc	87 [945; beta-D-Glucopyranose (5TMS)]	50	0.281	0.646	22.479	0.587	36	106	30	112	86	18 duplicate
13441	97 [756; beta-D-Methylgluc	28 Malic acid	52	0.281	0.574	16.003	0.421	38	104	35	107	28	106 duplicate
8962	97 [756; beta-D-Methylgluc	106 [733; Threitol (4TMS)]	50	0.257	0.461	15.780	0.602	39	103	43	99	26	11 original
8971	97 [756; beta-D-Methylgluc	115 Glucose-6-phosphate	51	0.255	0.544	15.973	0.576	40	102	38	104	27	26 original
12829	97 [756; beta-D-Methylgluc	21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.249	0.438	14.209	0.450	41	101	46	96	19	83 duplicate
15941	97 [756; beta-D-Methylgluc	53 Glycerol-2-phosphate	52	0.240	0.395	25.809	0.377	42	100	51	91	108	122 duplicate
17889	97 [756; beta-D-Methylgluc	78 Mannose	50	0.236	0.469	19.398	0.463	43	99	42	100	59	75 duplicate
8976	97 [756; beta-D-Methylgluc	120 [945; Uridine (3TMS)]	49	0.235	0.196	16.043	0.441	44	98	63	79	30	89 original
17762	97 [756; beta-D-Methylgluc	76 Fructose	52	0.232	0.594	15.736	0.518	45	96	33	109	25	54 duplicate
13214	97 [756; beta-D-Methylgluc	26 Citramalic acid	52	0.232	0.398	14.897	0.422	46	97	50	92	22	105 duplicate
16839	97 [756; beta-D-Methylgluc	63 Glutamine	40	0.228	-0.371	30.463	0.579	47	95	100	42	130	21 duplicate
8956	97 [756; beta-D-Methylgluc	100 [857; Mannitol (6TMS)]	52	0.223	0.400	16.800	0.441	48	94	49	93	41	91 original
8973	97 [756; beta-D-Methylgluc	117 [724; Glycerol (3TMS)]	49	0.218	0.334	20.196	0.493	49	93	55	87	65	66 original
18302	97 [756; beta-D-Methylgluc	85 [529; Methylcitric acid (4TMS)]	36	0.210	0.318	9.648	0.446	50	92	56	86	4	86 duplicate
15853	97 [756; beta-D-Methylgluc	52 [NA]	34	0.209	-0.280	35.092	0.637	51	91	94	48	138	6 duplicate
8968	97 [756; beta-D-Methylgluc	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	52	0.208	0.310	30.211	0.417	52	90	57	85	129	107 original
14719	97 [756; beta-D-Methylgluc	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	51	0.198	0.418	22.001	0.469	53	89	48	94	83	73 duplicate
17564	97 [756; beta-D-Methylgluc	73 [708; Glucose methoxymamine (5TMS)]	45	0.198	0.286	17.638	0.425	54	88	59	83	45	102 duplicate
8978	97 [756; beta-D-Methylgluc	122 [644; Erythritol (4TMS)]	50	0.193	0.395	27.510	0.517	55	87	52	90	115	55 original
8966	97 [756; beta-D-Methylgluc	110 [715; Erythritol (4TMS)]	49	0.192	0.293	21.732	0.640	56	86	58	84	79	5 original
8991	97 [756; beta-D-Methylgluc	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	52	0.189	0.213	16.015	0.366	57	85	62	80	29	128 original
14204	97 [756; beta-D-Methylgluc	35 Pyroglutamic acid	52	0.164	0.558	27.401	0.516	58	84	37	105	113	57 duplicate
18567	97 [756; beta-D-Methylgluc	90 [910; 9-(2)-Hexadecenoic acid (1TMS)]	52	0.155	0.162	19.524	0.392	59	83	67	75	60	117 duplicate
8958	97 [756; beta-D-Methylgluc	102 [904; Galactose methoxymamine (5TMS)]	52	0.151	0.260	21.555	0.411	60	82	60	82	75	110 original
8977	97 [756; beta-D-Methylgluc	121 [657; Erythritol (4TMS)]	48	0.144	0.178	26.884	0.451	61	81	64	78	110	80 original
15113	97 [756; beta-D-Methylgluc	44 [910; 2-Ketogluconic acid methoxymamine (4TMS)]	48	0.115	0.150	18.236	0.560	62	80	68	74	48	36 duplicate
18012	97 [756; beta-D-Methylgluc	80 [772; D-Glucose (5TMS)]	50	0.099	0.514	19.181	0.543	63	79	40	102	56	45 duplicate
10724	97 [756; beta-D-Methylgluc	6 Glycerol	52	0.094	0.424	27.944	0.563	64	78	47	95	120	31 duplicate
8972	97 [756; beta-D-Methylgluc	116 [882; Pseudouridine (5TMS)]	24	0.087	0.029	12.841	0.376	65	77	71	71	16	128 original
8981	97 [756; beta-D-Methylgluc	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru	52	0.083	0.559	20.509	0.546	66	76	36	106	66	44 original
8975	97 [756; beta-D-Methylgluc	119 [931; myo-Inositol-2-phosphate (7TMS)]	52	0.057	-0.006	20.848	0.379	67	75	74	68	69	121 original
8988	97 [756; beta-D-Methylgluc	132 [895; Isomaltose methoxymamine (8TMS)]	39	0.053	0.469	24.745	0.429	68	74	41	101	100	99 original
12266	97 [756; beta-D-Methylgluc	18 [590; 1-Acetyl-2-thiohydantoin]	52	0.042	0.088	18.420	0.377	69	73	69	73	49	125 duplicate
8982	97 [756; beta-D-Methylgluc	128 [559; Erythritol (4TMS)]	45	0.040	-0.011	22.905	0.573	70	72	76	68	91	27 original
15016	97 [756; beta-D-Methylgluc	43 [546; Leucine (2TBS)]	48	0.039	-0.016	18.425	0.369	71	71	78	64	50	128 duplicate
18516	97 [756; beta-D-Methylgluc	89 [775; Dopamine (4TMS)]	23	0.036	-0.588	25.199	0.532	72	70	115	27	104	48 duplicate

8963	97 [756; beta-D-Methylgluc	107	9-(Z)-Octadecenoic acid	52	0.002	-0.140	16,525	0.425	73	69	87	55	38	101	original
8998	97 [756; beta-D-Methylgluc	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	37	0.000	0.008	24,924	0.328	74	67	73	69	101	135	original
8992	97 [756; beta-D-Methylgluc	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.000	-0.274	12,612	0.422	75	68	93	49	14	104	original
17631	97 [756; beta-D-Methylgluc	74	[912; Tetradecanoic acid (1TMS)]	52	-0.017	0.044	22,616	0.399	76	68	70	72	88	114	duplicate
18552	97 [756; beta-D-Methylgluc	96	myo-Inositol	37	-0.024	-0.011	27,641	0.265	77	65	77	65	117	140	duplicate
17496	97 [756; beta-D-Methylgluc	72	[919; D-Xylopyranose (4TMS)]	51	-0.035	-0.009	23,228	0.364	78	64	75	67	92	119	duplicate
18807	97 [756; beta-D-Methylgluc	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	38	-0.036	-0.329	33,579	0.408	79	63	97	45	135	111	duplicate
15583	97 [756; beta-D-Methylgluc	49	[877; Pyrophosphoric acid (4TMS)]	52	-0.036	-0.020	34,496	0.406	80	62	79	63	137	112	duplicate
8967	97 [756; beta-D-Methylgluc	111	[583; Erythritol (4TMS)]	38	-0.050	-0.101	31,704	0.308	81	61	84	58	133	138	original
8969	97 [756; beta-D-Methylgluc	113	Galactose-6-phosphate	51	-0.053	0.345	20,520	0.646	82	60	54	88	67	3	original
8997	97 [756; beta-D-Methylgluc	141	Lanosta-8,24-dien-3-beta-ol	49	-0.061	-0.115	27,372	0.377	83	59	86	56	112	123	original
14819	97 [756; beta-D-Methylgluc	41	[639; Proline (2TMS)]	52	-0.074	0.028	16,202	0.495	84	58	72	70	33	65	duplicate
12388	97 [756; beta-D-Methylgluc	19	Alanine (BP) (3TMS)	52	-0.090	0.168	16,162	0.559	85	57	65	77	32	38	duplicate
8974	97 [756; beta-D-Methylgluc	118	[928; Glucopyranose-6-phosphate (6TMS)]	50	-0.118	-0.041	22,488	0.441	86	56	81	61	87	90	original
8970	97 [756; beta-D-Methylgluc	114	Fructose-6-phosphate	44	-0.118	0.246	21,716	0.642	87	55	61	81	78	4	original
8995	97 [756; beta-D-Methylgluc	139	[700; Ergosta-5,7-dien-3-ol]	30	-0.122	-0.173	27,412	0.293	88	54	88	54	114	139	original
8960	97 [756; beta-D-Methylgluc	104	[795; Erythritol (4TMS)]	51	-0.126	-0.036	19,753	0.539	89	53	80	62	62	48	original
16682	97 [756; beta-D-Methylgluc	61	[NA]	52	-0.127	-0.291	21,561	0.467	90	52	95	47	76	74	duplicate
18761	97 [756; beta-D-Methylgluc	94	Hexadecanoic acid	52	-0.140	-0.210	19,281	0.470	91	51	90	52	58	72	duplicate
8965	97 [756; beta-D-Methylgluc	133	[855; Squalene]	52	-0.145	-0.306	21,920	0.377	93	50	96	46	82	124	original
8989	97 [756; beta-D-Methylgluc	45	Homocysteine	49	-0.168	-0.240	35,321	0.382	94	48	91	51	139	120	duplicate
15209	97 [756; beta-D-Methylgluc	25	[709; 2,5-Diaminovalerolactam (2TMS)]	47	-0.169	-0.564	30,923	0.509	95	47	112	30	131	60	duplicate
13099	97 [756; beta-D-Methylgluc	48	Asparagine	46	-0.171	-0.493	19,873	0.455	96	46	104	38	63	77	duplicate
18189	97 [756; beta-D-Methylgluc	83	Sorbitol	52	-0.183	-0.112	21,084	0.442	97	45	85	67	71	88	duplicate
16916	97 [756; beta-D-Methylgluc	64	[789; Tyramine (3TMS)]	52	-0.189	-0.060	17,023	0.625	98	44	83	59	42	7	original
8979	97 [756; beta-D-Methylgluc	123	[945; Galactofuranose-6-phosphate (7TMS)]	52	-0.205	-0.052	16,634	0.563	99	43	82	60	39	32	duplicate
18694	97 [756; beta-D-Methylgluc	15	Alanine	52	-0.205	-0.390	21,499	0.325	100	42	102	40	73	136	original
8993	97 [756; beta-D-Methylgluc	137	Ergosterol	52	-0.210	-0.357	36,770	0.388	101	41	99	43	141	118	original
8980	97 [756; beta-D-Methylgluc	124	[734; 1-Monooctadecylglycerol (2TMS); 1-Monooctadecylglycerol (2TMS)]	47	-0.214	-0.357	36,770	0.388	101	41	99	43	141	118	original
8987	97 [756; beta-D-Methylgluc	131	[626; 5-Methylthiodenosine (3TMS)]	44	-0.230	-0.252	30,032	0.530	102	40	92	50	128	50	original
15491	97 [756; beta-D-Methylgluc	48	Asparagine	52	-0.238	-0.547	25,709	0.549	103	39	108	34	106	43	duplicate
8994	97 [756; beta-D-Methylgluc	138	[674; Ergosterol (1TMS)]	36	-0.241	-0.350	28,460	0.463	104	38	98	44	125	76	original
17951	97 [756; beta-D-Methylgluc	79	Glucose	52	-0.261	0.166	23,880	0.661	105	37	66	76	94	2	duplicate
12509	97 [756; beta-D-Methylgluc	20	[619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	19	-0.310	-0.806	18,532	0.444	106	36	137	5	51	87	duplicate
18131	97 [756; beta-D-Methylgluc	82	Lysine	27	-0.316	-0.712	15,806	0.525	107	35	129	13	24	51	duplicate
8986	97 [756; beta-D-Methylgluc	130	Trehalose	52	-0.323	-0.373	20,145	0.395	108	33	101	41	64	116	original
12866	97 [756; beta-D-Methylgluc	23	Homoserine	52	-0.323	-0.567	25,049	0.454	109	34	113	29	103	78	duplicate
13328	97 [756; beta-D-Methylgluc	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	41	-0.332	-0.586	31,162	0.368	110	32	114	28	132	131	duplicate
8964	97 [756; beta-D-Methylgluc	108	Octadecenoic acid	52	-0.332	-0.555	24,673	0.412	111	31	109	33	98	109	original
15764	97 [756; beta-D-Methylgluc	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	32	-0.351	-0.655	28,111	0.372	112	30	121	21	122	127	duplicate
17427	97 [756; beta-D-Methylgluc	123	[931; Erythrose (3TMS)]	52	-0.354	-0.559	17,824	0.424	113	29	111	31	44	103	duplicate
14098	97 [756; beta-D-Methylgluc	34	Aspartic acid	52	-0.359	-0.497	23,631	0.322	114	28	105	37	93	137	duplicate
8954	97 [756; beta-D-Methylgluc	98	[697; Ribose-5-phosphate methoxamine (5TMS)]	37	-0.360	-0.557	33,093	0.355	115	27	110	32	134	132	original
16439	97 [756; beta-D-Methylgluc	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	52	-0.373	-0.595	20,857	0.488	116	26	116	28	70	68	duplicate
10453	97 [756; beta-D-Methylgluc	4	Phosphoric acid	40	-0.374	-0.497	24,694	0.398	117	25	108	36	99	115	duplicate
16114	97 [756; beta-D-Methylgluc	55	[612; 4-Aminobutyric acid (2TBS)]	31	-0.381	-0.822	27,809	0.533	118	24	140	2	118	47	duplicate
17214	97 [756; beta-D-Methylgluc	68	[570; Hypoxanthine (2TMS)]	11	-0.382	-0.820	19,689	0.251	119	23	139	3	61	141	duplicate
10589	97 [756; beta-D-Methylgluc	5	Leucine	33	-0.383	-0.472	18,463	0.348	120	22	103	39	35	133	duplicate

13981	97 [756; beta-D-Methylgluc 33	Methionine	52	-0.391	-0.511	25,009	0.338	121	21	107	35	102	134 duplicate
10991	97 [756; beta-D-Methylgluc 8	Isoleucine	43	-0.391	-0.633	22,811	0.401	122	20	118	24	90	113 duplicate
17697	97 [756; beta-D-Methylgluc 75	Lysine	52	-0.392	-0.647	27,820	0.495	123	19	119	23	118	64 duplicate
17286	97 [756; beta-D-Methylgluc 69	Arginine	48	-0.399	-0.665	21,890	0.492	124	18	123	19	81	67 duplicate
17826	97 [756; beta-D-Methylgluc 77	benzeneacetic acid methyl ester]	50	-0.407	-0.753	25,538	0.434	125	17	133	9	105	97 duplicate
16521	97 [756; beta-D-Methylgluc 59	Ornithine; Arginine	52	-0.430	-0.654	28,122	0.439	126	16	120	22	123	94 duplicate
13664	97 [756; beta-D-Methylgluc 30	[815; Ethyl-3(2H)-thiophenone]	52	-0.442	-0.597	24,416	0.366	127	15	117	25	97	130 duplicate
14309	97 [756; beta-D-Methylgluc 38	[596; N-Acetylglutamic acid (2TMS)]	52	-0.448	-0.700	22,409	0.530	128	14	126	16	84	49 duplicate
13774	97 [756; beta-D-Methylgluc 31	[622; Parabanic acid (2TMS)]	52	-0.454	-0.658	28,044	0.433	129	12	122	20	121	98 duplicate
11254	97 [756; beta-D-Methylgluc 10	Glycine	52	-0.454	-0.757	20,598	0.561	130	13	135	7	68	35 duplicate
10178	97 [756; beta-D-Methylgluc 2	Serine	50	-0.458	-0.690	26,394	0.435	131	11	125	17	108	98 duplicate
17141	97 [756; beta-D-Methylgluc 67	Citric acid	52	-0.472	-0.739	17,612	0.440	132	10	130	12	43	93 duplicate
10858	97 [756; beta-D-Methylgluc 7	Threonine	52	-0.481	-0.686	21,185	0.426	133	8	124	18	72	100 duplicate
14413	97 [756; beta-D-Methylgluc 37	Phenylalanine	52	-0.481	-0.757	18,017	0.521	134	9	134	8	46	52 duplicate
13883	97 [756; beta-D-Methylgluc 32	[729; N,N-Dimethyllysine methyl ester]	51	-0.487	-0.743	33,686	0.478	135	7	131	11	136	71 duplicate
14918	97 [756; beta-D-Methylgluc 42	Glutamic acid	48	-0.498	-0.709	27,518	0.416	136	6	128	14	116	108 duplicate
11123	97 [756; beta-D-Methylgluc 9	Proline	51	-0.504	-0.709	26,255	0.451	137	5	127	15	124	82 duplicate
16602	97 [756; beta-D-Methylgluc 60	Glycerol-3-phosphate	52	-0.516	-0.795	18,757	0.579	138	4	136	6	53	22 duplicate
10316	97 [756; beta-D-Methylgluc 3	Ethanolamine	50	-0.523	-0.818	29,034	0.591	139	3	138	4	126	14 duplicate
17067	97 [756; beta-D-Methylgluc 66	Glycine acid-3-phosphate	52	-0.538	-0.746	24,213	0.503	140	2	132	10	95	63 duplicate
18072	97 [756; beta-D-Methylgluc 81	Tyrosine	52	-0.560	-0.923	25,792	0.690	141	1	141	1	107	1 duplicate
12867	98 [697; Ribose-5-phospha 23	Homoserine	48	0.599	0.821	19,209	0.584	1	141	3	139	64	13 duplicate
17215	98 [697; Ribose-5-phospha 68	[570; Hypoxanthine (2TMS)]	16	0.583	0.891	3,540	0.531	2	140	1	141	1	38 duplicate
13100	98 [697; Ribose-5-phospha 25	[709; 2,5-Diaminovalerolactam (2TMS)]	35	0.543	0.828	13,344	0.433	3	139	2	140	32	93 duplicate
11124	98 [697; Ribose-5-phospha 2	Proline	47	0.530	0.547	35,251	0.465	4	137	26	116	118	75 duplicate
10179	98 [697; Ribose-5-phospha 2	Serine	47	0.530	0.543	26,575	0.483	5	138	27	115	94	66 duplicate
13982	98 [697; Ribose-5-phospha 33	Methionine	48	0.527	0.652	19,091	0.543	6	136	15	127	63	33 duplicate
13329	98 [697; Ribose-5-phospha 27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	41	0.515	0.769	9,107	0.641	7	135	6	136	12	3 duplicate
13775	98 [697; Ribose-5-phospha 31	[622; Parabanic acid (2TMS)]	48	0.500	0.689	11,151	0.503	8	134	13	129	20	54 duplicate
17088	98 [697; Ribose-5-phospha 68	Glyceric acid-3-phosphate	48	0.482	0.638	14,714	0.495	9	133	17	125	36	59 duplicate
13685	98 [697; Ribose-5-phospha 30	[815; Ethyl-3(2H)-thiophenone]	48	0.466	0.603	39,418	0.475	10	132	19	123	126	72 duplicate
13884	98 [697; Ribose-5-phospha 32	[729; N,N-Dimethyllysine methyl ester]	48	0.459	0.730	12,691	0.630	11	131	9	133	29	6 duplicate
18517	98 [697; Ribose-5-phospha 89	[775; Dopamine (4TMS)]	26	0.458	0.634	11,507	0.498	12	130	18	124	22	66 duplicate
11255	98 [697; Ribose-5-phospha 10	Glycine	48	0.450	0.795	29,814	0.567	13	129	5	137	105	19 duplicate
10982	98 [697; Ribose-5-phospha 8	Isoleucine	42	0.449	0.401	25,788	0.436	14	128	39	103	92	91 duplicate
16840	98 [697; Ribose-5-phospha 63	Glutamine	37	0.423	0.590	16,506	0.486	15	127	20	122	44	60 duplicate
9030	98 [697; Ribose-5-phospha 131	[626; 5-Methylthioadenosine (3TMS)]	45	0.416	0.729	6,217	0.478	16	128	10	132	3	71 original
18073	98 [697; Ribose-5-phospha 81	Tyrosine	48	0.408	0.555	42,878	0.553	17	124	14	128	133	28 duplicate
14099	98 [697; Ribose-5-phospha 34	Aspartic acid	48	0.408	0.518	42,705	0.518	18	125	30	112	132	44 duplicate
17287	98 [697; Ribose-5-phospha 69	Arginine	45	0.406	0.748	30,114	0.639	19	123	7	135	110	5 duplicate
17698	98 [697; Ribose-5-phospha 75	Lysine	48	0.402	0.524	48,411	0.410	20	122	29	113	138	104 duplicate
16522	98 [697; Ribose-5-phospha 59	Ornithine; Arginine	48	0.399	0.582	49,662	0.512	21	121	23	119	139	48 duplicate
15492	98 [697; Ribose-5-phospha 48	Asparagine	48	0.397	0.652	18,977	0.482	22	120	16	128	62	68 duplicate
14414	98 [697; Ribose-5-phospha 37	Phenylalanine	48	0.394	0.578	33,702	0.449	23	119	24	118	116	84 duplicate
15210	98 [697; Ribose-5-phospha 45	Homocysteine	47	0.391	0.529	6,955	0.481	24	118	28	114	5	70 duplicate
10859	98 [697; Ribose-5-phospha 7	Threonine	48	0.383	0.514	40,157	0.450	25	117	31	111	128	83 duplicate
14819	98 [697; Ribose-5-phospha 42	Glutamic acid	46	0.378	0.703	37,220	0.548	26	116	12	130	122	31 duplicate
16440	98 [697; Ribose-5-phospha 58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	48	0.365	0.425	26,838	0.393	27	115	37	105	97	110 duplicate
15765	98 [697; Ribose-5-phospha 51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	35	0.355	0.801	5,106	0.608	28	114	4	138	2	8 duplicate

10317	98 [697; Ribose-5-phosphat	3	Ethanolamine	48	0.346	0.586	11.595	0.458	28	113	21	121	23	79 duplicate
14310	98 [697; Ribose-5-phosphat	36	[596; N-Acetylglutamic acid (2TMS)]	48	0.340	0.570	36.334	0.465	30	112	25	117	124	73 duplicate
18132	98 [697; Ribose-5-phosphat	82	Lysine	29	0.335	0.735	22.758	0.645	31	111	8	134	80	2 duplicate
17827	98 [697; Ribose-5-phosphat	77	[826; beta-[[[5-methyl-2-thienyl]methyl]eneamino-benzeneacetic acid methyl ester]	47	0.330	0.583	38.132	0.510	32	110	22	120	123	50 duplicate
15017	98 [697; Ribose-5-phosphat	43	[548; Leucine (2TBS)]	45	0.305	0.460	16.277	0.415	33	109	34	108	60	102 duplicate
16883	98 [697; Ribose-5-phosphat	61	[NA]	48	0.300	0.326	17.723	0.370	34	108	42	100	55	118 duplicate
15584	98 [697; Ribose-5-phosphat	49	[877; Pyrophosphoric acid (4TMS)]	48	0.294	0.470	10.489	0.407	35	107	33	109	18	106 duplicate
15854	98 [697; Ribose-5-phosphat	52	[NA]	35	0.291	0.460	9.852	0.515	36	106	35	107	16	47 duplicate
10454	98 [697; Ribose-5-phosphat	4	Phosphoric acid	37	0.279	0.430	39.140	0.442	37	105	36	106	125	77 duplicate
17142	98 [697; Ribose-5-phosphat	67	Citric acid	48	0.262	0.403	34.844	0.401	38	104	38	104	117	107 duplicate
9029	98 [697; Ribose-5-phosphat	130	Trehalose	47	0.258	0.470	40.099	0.359	39	103	32	110	127	124 original
18180	98 [697; Ribose-5-phosphat	83	Sorbitol	43	0.243	0.283	29.986	0.462	40	102	45	97	108	77 duplicate
16603	98 [697; Ribose-5-phosphat	60	Glycerol-3-phosphate	48	0.225	0.380	32.385	0.440	41	101	40	102	114	88 duplicate
9007	98 [697; Ribose-5-phosphat	108	Octadecanoic acid	48	0.172	0.388	14.866	0.361	42	100	41	101	37	122 original
10590	98 [697; Ribose-5-phosphat	5	Leucine	33	0.159	0.720	10.121	0.728	43	99	11	131	17	1 duplicate
16115	98 [697; Ribose-5-phosphat	55	[612; 4-Aminobutyric acid (2TBS)]	32	0.145	0.300	9.358	0.558	44	98	43	99	14	25 duplicate
18808	98 [697; Ribose-5-phosphat	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	42	0.143	0.241	7.888	0.431	45	97	46	98	8	95 duplicate
16917	98 [697; Ribose-5-phosphat	64	[789; Tyramine (3TMS)]	47	0.121	0.047	16.531	0.338	46	96	54	88	45	126 duplicate
17428	98 [697; Ribose-5-phosphat	71	[731; Erythrose (3TMS)]	48	0.105	0.069	24.403	0.485	47	95	53	89	85	61 duplicate
11895	98 [697; Ribose-5-phosphat	15	Alanine	48	0.082	-0.013	29.835	0.540	48	94	55	87	106	34 duplicate
10040	98 [697; Ribose-5-phosphat	1	[938; Sulfuric acid (2TMS)]	23	0.075	-0.197	17.365	0.334	49	93	61	81	51	128 duplicate
9032	98 [697; Ribose-5-phosphat	133	[855; Squalene]	48	0.016	-0.217	44.445	0.438	50	92	65	77	137	89 duplicate
17497	98 [697; Ribose-5-phosphat	72	[919; D-Xylopyranose (4TMS)]	48	0.014	0.072	18.269	0.337	51	91	52	90	59	127 original
9006	98 [697; Ribose-5-phosphat	107	[9-(Z)-Octadecanoic acid	48	0.012	0.109	16.402	0.311	52	90	50	82	43	135 duplicate
	98 [697; Ribose-5-phosphat	124	[734; 1-Monoololeoylglycerol (2TMS); 1-Monohexadecenoylethanolamine (1TMS)]	48	-0.005	0.175	26.586	0.298	53	89	47	95	95	136 original
9023	98 [697; Ribose-5-phosphat	53	Glycerol-2-phosphate	45	-0.024	0.091	9.272	0.316	54	88	51	91	13	133 original
15942	98 [697; Ribose-5-phosphat	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	48	-0.030	0.161	11.879	0.373	55	87	48	94	24	117 duplicate
9035	98 [697; Ribose-5-phosphat	104	[785; Erythritol (4TMS)]	9	-0.056	-0.196	12.201	0.125	56	86	60	82	26	141 original
9003	98 [697; Ribose-5-phosphat	123	[945; Galactofuranose-6-phosphate (7TMS)]	47	-0.077	-0.234	17.574	0.484	57	85	87	75	53	82 original
9022	98 [697; Ribose-5-phosphat	6	Glycerol	48	-0.078	-0.256	23.197	0.409	58	84	68	74	82	105 original
10725	98 [697; Ribose-5-phosphat	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	48	-0.089	-0.380	50.462	0.413	59	83	72	70	141	103 duplicate
18568	98 [697; Ribose-5-phosphat	137	Ergosterol	48	-0.108	-0.016	19.643	0.284	60	82	56	86	65	138 duplicate
9036	98 [697; Ribose-5-phosphat	139	[700; Ergosta-5,7-dien-3-ol]	48	-0.110	0.126	24.515	0.327	61	81	49	93	86	131 original
9038	98 [697; Ribose-5-phosphat	111	[583; Erythritol (4TMS)]	26	-0.114	-0.089	7.008	0.200	62	80	58	84	6	140 original
9010	98 [697; Ribose-5-phosphat	119	[931; myo-Inositol-2-phosphate (7TMS)]	27	-0.123	-0.200	7.316	0.314	63	79	62	80	7	134 original
9017	98 [697; Ribose-5-phosphat	118	[928; Glucopyranose-6-phosphate (6TMS)]	48	-0.135	-0.131	20.053	0.330	64	78	59	83	67	130 original
12267	98 [697; Ribose-5-phosphat	18	[590; 1-Acetyl-2-thiohydantoin]	42	-0.141	-0.223	16.980	0.284	65	77	66	76	49	137 original
17565	98 [697; Ribose-5-phosphat	138	[674; Ergosterol (1TMS)]	48	-0.160	-0.349	20.056	0.424	66	76	71	71	69	97 duplicate
9037	98 [697; Ribose-5-phosphat	73	[708; Glucose methoxyamine (5TMS)]	43	-0.169	-0.529	16.613	0.484	67	75	84	58	46	63 duplicate
12389	98 [697; Ribose-5-phosphat	19	Alanine [BP] (3TMS)	32	-0.185	-0.206	8.790	0.370	68	74	64	78	10	119 original
9024	98 [697; Ribose-5-phosphat	125	[892; Sucrose (6TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	48	-0.186	-0.429	23.777	0.446	69	73	75	67	84	86 duplicate
9012	98 [697; Ribose-5-phosphat	113	Galactose-6-phosphate	48	-0.188	-0.468	41.789	0.386	70	72	78	64	130	113 original
	98 [697; Ribose-5-phosphat	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	46	-0.188	-0.522	16.672	0.393	71	71	83	59	47	111 original
12510	98 [697; Ribose-5-phosphat	41	[639; Proline (2TMS)]	23	-0.202	0.293	6.298	0.640	72	70	44	98	4	4 duplicate
14820	98 [697; Ribose-5-phosphat	94	Hexadecanoic acid	48	-0.204	-0.384	25.494	0.458	73	69	73	69	91	80 duplicate
18762	98 [697; Ribose-5-phosphat	109	Octadecanoic acid	48	-0.209	-0.430	31.820	0.433	74	67	76	66	113	94 duplicate
9008	98 [697; Ribose-5-phosphat	29	Erythritol	48	-0.209	-0.494	31.065	0.417	75	68	80	62	112	99 original
13554	98 [697; Ribose-5-phosphat	109	Erythritol	48	-0.216	-0.739	17.618	0.596	76	66	116	26	54	11 duplicate

18013	98 [697; Ribose-5-phosphat	80	[772; D-Glucose (5TMS)]	47	-0.219	-0.437	41,249	0.385	77	65	77	65	129	115-juplicate
18618	98 [697; Ribose-5-phosphat	91	[766; beta-D-Methylglucopyranoside (4TMS)]	48	-0.222	-0.520	28,114	0.510	78	64	82	60	98	51-juplicate
9019	98 [697; Ribose-5-phosphat	120	[945; Uridine (3TMS)]	39	-0.223	-0.305	23,018	0.557	79	63	57	85	81	26 original
8998	98 [697; Ribose-5-phosphat	99	[662; Ribose-5-phosphat methoxyamine (BP) (5TMS)]	27	-0.231	-0.708	15,581	0.367	80	62	111	31	40	120 original
12144	98 [697; Ribose-5-phosphat	17	[700; 2-methyl-1,2-propanediol (2TMS)]	48	-0.239	-0.678	29,885	0.483	81	61	103	39	107	65-juplicate
11365	98 [697; Ribose-5-phosphat	11	Succinic acid	48	-0.254	-0.663	20,598	0.515	82	60	98	44	70	46-juplicate
18412	98 [697; Ribose-5-phosphat	87	[945; beta-D-Glucopyranose (5TMS)]	46	-0.258	-0.496	44,157	0.421	83	59	81	61	135	98-juplicate
9040	98 [697; Ribose-5-phosphat	141	Lanosta-8,24-dien-3-beta-ol	45	-0.261	-0.267	11,502	0.395	84	57	69	73	21	109 original
18358	98 [697; Ribose-5-phosphat	86	[793; D-Galactono-1,4-lactone (4TMS)]	45	-0.261	-0.703	30,773	0.594	85	58	109	33	111	12-juplicate
12630	98 [697; Ribose-5-phosphat	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	48	-0.266	-0.562	28,515	0.517	86	56	90	52	101	45-juplicate
18653	98 [697; Ribose-5-phosphat	96	myo-Inositol	38	-0.266	-0.322	8,800	0.365	87	55	70	72	11	121-juplicate
15399	98 [697; Ribose-5-phosphat	47	[NA]	48	-0.270	-0.204	21,427	0.428	88	54	63	79	74	96-juplicate
12020	98 [697; Ribose-5-phosphat	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	48	-0.275	-0.772	30,080	0.603	89	53	127	15	109	9-juplicate
12984	98 [697; Ribose-5-phosphat	24	[725; 2-Ketooctanoic acid (2TMS)]	48	-0.280	-0.765	42,235	0.578	90	52	130	12	131	15-juplicate
17358	98 [697; Ribose-5-phosphat	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	42	-0.282	-0.539	28,964	0.400	91	51	85	57	103	108-juplicate
14517	98 [697; Ribose-5-phosphat	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	48	-0.298	-0.826	20,797	0.559	92	50	137	5	72	24-juplicate
15305	98 [697; Ribose-5-phosphat	46	Arabinose	48	-0.301	-0.748	29,047	0.535	93	49	121	21	104	36-juplicate
16993	98 [697; Ribose-5-phosphat	65	[646; 3-Deoxyglucitol (5TMS)]	47	-0.306	-0.784	22,150	0.531	94	48	128	13	77	38-juplicate
9013	98 [697; Ribose-5-phosphat	114	Fructose-6-phosphate	37	-0.306	-0.823	15,276	0.392	95	47	84	48	38	112 original
13215	98 [697; Ribose-5-phosphat	26	Citramalic acid	48	-0.309	-0.663	28,408	0.529	96	46	100	42	100	41-juplicate
16029	98 [697; Ribose-5-phosphat	54	[NA]	40	-0.313	-0.691	16,906	0.415	97	45	106	36	48	101-juplicate
9000	98 [697; Ribose-5-phosphat	101	[832; Dopamine (4TMS)]	48	-0.314	-0.819	23,424	0.482	98	44	93	49	83	67 original
18715	98 [697; Ribose-5-phosphat	93	[607; Putrescine (4TMS)]	44	-0.315	-0.613	14,353	0.416	99	43	79	63	35	100-juplicate
16273	98 [697; Ribose-5-phosphat	56	[829; Oroic acid (3TMS)]	48	-0.319	-0.759	20,056	0.523	100	42	125	17	68	43-juplicate
16762	98 [697; Ribose-5-phosphat	62	[812; D-Xylofuranose (4TMS)]	48	-0.321	-0.691	26,777	0.508	101	41	105	37	96	52-juplicate
18247	98 [697; Ribose-5-phosphat	84	Mannitol	47	-0.321	-0.539	42,916	0.461	102	39	86	56	134	78-juplicate
14819	98 [697; Ribose-5-phosphat	39	[829; 1-Phenylethanol (1TMS)]	47	-0.321	-0.823	28,207	0.560	103	40	136	6	99	22-juplicate
17890	98 [697; Ribose-5-phosphat	78	Mannose	46	-0.328	-0.831	18,105	0.465	104	38	98	46	57	74-juplicate
18465	98 [697; Ribose-5-phosphat	88	Gluconic acid	48	-0.328	-0.733	24,884	0.559	105	37	115	27	89	23-juplicate
13442	98 [697; Ribose-5-phosphat	28	Malic acid	48	-0.340	-0.822	22,205	0.599	106	36	135	7	78	10-juplicate
9033	98 [697; Ribose-5-phosphat	134	Isomaltose	48	-0.344	-0.794	36,217	0.563	108	34	132	10	121	20 original
9028	98 [697; Ribose-5-phosphat	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	44	-0.345	-0.771	22,479	0.497	109	33	126	16	79	58 original
16357	98 [697; Ribose-5-phosphat	57	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	40	-0.346	-0.719	25,244	0.453	110	32	112	30	90	81-juplicate
9001	98 [697; Ribose-5-phosphat	102	[904; Galactose methoxyamine (5TMS)]	48	-0.353	-0.616	16,020	0.500	111	31	92	50	42	55 original
14205	98 [697; Ribose-5-phosphat	35	Pyroglutamic acid	48	-0.355	-0.627	50,003	0.433	112	29	95	47	140	92-juplicate
11642	98 [697; Ribose-5-phosphat	13	Uracil	48	-0.355	-0.796	28,733	0.592	113	30	133	9	102	14-juplicate
9002	98 [697; Ribose-5-phosphat	103	[646; Ethylamine (2TMS)]	47	-0.358	-0.704	26,458	0.547	114	28	110	32	93	32 original
18697	98 [697; Ribose-5-phosphat	97	[756; beta-D-Methylglucopyranoside (4TMS)]	37	-0.360	-0.557	33,093	0.355	115	27	88	54	115	125-juplicate
11769	98 [697; Ribose-5-phosphat	14	Fumaric acid	48	-0.362	-0.792	14,202	0.574	116	26	131	11	34	16-juplicate
15675	98 [697; Ribose-5-phosphat	50	[746; Ribonic acid-1,4-lactone (3TMS)]	45	-0.364	-0.753	12,128	0.556	117	25	123	19	25	27-juplicate
11514	98 [697; Ribose-5-phosphat	12	Glycic acid	47	-0.367	-0.749	13,318	0.535	118	24	122	20	31	37-juplicate
18303	98 [697; Ribose-5-phosphat	85	[529; Methylcitric acid (4TMS)]	35	-0.368	-0.692	12,611	0.625	119	23	107	35	27	7-juplicate
9034	98 [697; Ribose-5-phosphat	135	[902; Maltose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	48	-0.369	-0.652	24,793	0.437	120	22	97	45	88	90 original
9011	98 [697; Ribose-5-phosphat	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (8TMS)]	47	-0.380	-0.686	9,532	0.482	121	21	104	38	15	69 original
9014	98 [697; Ribose-5-phosphat	115	Glucose-6-phosphate	46	-0.389	-0.668	35,474	0.447	122	20	101	41	119	85 original
14720	98 [697; Ribose-5-phosphat	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	48	-0.392	-0.741	44,186	0.561	123	19	117	25	136	21-juplicate
9039	98 [697; Ribose-5-phosphat	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	34	-0.401	-0.386	8,570	0.383	124	18	74	68	9	116 original
17632	98 [697; Ribose-5-phosphat	74	[912; Tetradecanoic acid (1TMS)]	48	-0.411	-0.674	18,307	0.530	125	17	102	40	61	40-juplicate

17763	98 [697; Ribose-5-phospha	76	Fructose	48	-0.418	-0.663	35.965	0.540	126	16	99	43	120	35 duplicate
12749	98 [697; Ribose-5-phospha	22	[690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	39	-0.436	-0.841	13.763	0.548	127	15	139	3	33	29 duplicate
9005	98 [697; Ribose-5-phospha	106	[733; Threitol (4TMS)]	46	-0.451	-0.743	21.775	0.571	128	14	118	24	75	18 original
8899	98 [697; Ribose-5-phospha	100	[657; Mannitol (6TMS)]	48	-0.454	-0.747	21.872	0.512	129	13	120	22	76	49 original
18667	98 [697; Ribose-5-phospha	92	[680; Glycerol-2-phosphate (4TMS)]	40	-0.459	-0.570	19.819	0.332	130	12	91	51	66	129 duplicate
9004	98 [697; Ribose-5-phospha	105	[705; 2-Ketoglucuronic acid (5TMS)]	34	-0.465	-0.722	24.619	0.451	131	11	113	29	87	82 original
9026	98 [697; Ribose-5-phospha	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	25	-0.480	-0.701	17.549	0.326	132	10	108	34	52	132 original
9020	98 [697; Ribose-5-phospha	121	[657; Erythritol (4TMS)]	40	-0.495	-0.725	13.031	0.504	133	9	114	28	30	53 original
9031	98 [697; Ribose-5-phospha	132	[895; Isomaltose methoxyamine (8TMS)]	28	-0.508	-0.882	17.024	0.525	134	8	141	1	50	42 original
9015	98 [697; Ribose-5-phospha	116	[682; Pseudotriuridine (5TMS)]	19	-0.520	-0.559	12.682	0.278	135	7	89	53	28	139 original
15114	98 [697; Ribose-5-phospha	44	[910; 2-Ketoglucuronic acid methoxyamine (4TMS)]	35	-0.523	-0.755	20.599	0.464	136	6	124	18	71	76 duplicate
9027	98 [697; Ribose-5-phospha	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	31	-0.553	-0.745	21.298	0.385	137	5	119	23	73	114 original
9016	98 [697; Ribose-5-phospha	117	[724; Glycerol (3TMS)]	42	-0.554	-0.846	17.955	0.573	138	4	140	2	56	17 original
9009	98 [697; Ribose-5-phospha	110	[715; Erythritol (4TMS)]	40	-0.556	-0.783	18.225	0.548	139	3	128	14	59	30 original
9021	98 [697; Ribose-5-phospha	122	[644; Erythritol (4TMS)]	37	-0.559	-0.827	15.531	0.483	140	2	138	4	39	64 original
9025	98 [697; Ribose-5-phospha	128	[559; Erythritol (4TMS)]	31	-0.578	-0.811	15.776	0.497	141	1	134	8	41	57 original
9070	99 [662; Ribose-5-phospha		129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	41	0.768	0.943	10.175	0.645	1	140	5	136	37	16 original
9075	99 [662; Ribose-5-phospha	134	Isomaltose	41	0.761	0.929	27.371	0.663	2	139	10	131	120	8 original
15306	99 [662; Ribose-5-phospha	46	Arabinose	41	0.751	0.907	19.004	0.678	3	138	14	127	98	2 duplicate
16358	99 [662; Ribose-5-phospha		57 [757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	38	0.698	0.853	13.913	0.664	4	137	21	120	69	7 duplicate
12021	99 [662; Ribose-5-phospha	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	41	0.690	0.955	20.615	0.666	5	135	1	140	105	6 duplicate
11643	99 [662; Ribose-5-phospha	13	Uracil	41	0.690	0.953	19.216	0.666	6	136	2	139	99	5 duplicate
12985	99 [662; Ribose-5-phospha	24	[725; 2-Ketooctanoic acid (2TMS)]	41	0.688	0.952	32.864	0.652	7	134	4	137	133	13 duplicate
13555	99 [662; Ribose-5-phospha	29	Erythritol	41	0.685	0.953	8.740	0.655	8	133	3	138	23	11 duplicate
16274	99 [662; Ribose-5-phospha	56	[829; Orlic acid (3TMS)]	41	0.676	0.914	8.103	0.878	9	132	12	129	16	4 duplicate
14020	99 [662; Ribose-5-phospha	39	[829; 1-Phenylethanol (1TMS)]	41	0.673	0.933	18.939	0.650	10	130	7	134	97	9 duplicate
18468	99 [662; Ribose-5-phospha	88	Glucuronic acid	41	0.673	0.862	14.687	0.634	11	131	19	122	74	21 duplicate
15976	99 [662; Ribose-5-phospha	50	[746; Ribonic acid-1,4-lactone (3TMS)]	41	0.671	0.932	6.886	0.638	12	129	9	132	10	18 duplicate
12145	99 [662; Ribose-5-phospha	17	[700; 2-methyl-1,2-propanediol (2TMS)]	41	0.661	0.938	20.340	0.856	13	127	6	135	104	10 duplicate
16994	99 [662; Ribose-5-phospha	65	[646; 3-Deoxyglucitol (5TMS)]	41	0.661	0.919	9.761	0.882	14	128	11	130	31	1 duplicate
18998	99 [662; Ribose-5-phospha	97	[756; beta-D-Methylglucopyranoside (4TMS)]	39	0.625	0.792	21.529	0.591	15	126	27	114	109	37 duplicate
9046	99 [662; Ribose-5-phospha	105	[705; 2-Ketoglucuronic acid (5TMS)]	36	0.619	0.835	12.319	0.602	16	125	24	117	59	31 original
16030	99 [662; Ribose-5-phospha	54	[NA]	38	0.616	0.910	3.696	0.635	17	123	13	128	1	20 duplicate
18359	99 [662; Ribose-5-phospha	86	[793; D-Galactono-1,4-lactone (4TMS)]	38	0.616	0.857	22.924	0.637	18	124	20	121	111	19 duplicate
9044	99 [662; Ribose-5-phospha	103	[648; Ethylamine (2TMS)]	41	0.600	0.788	15.380	0.519	19	122	26	115	80	62 original
18668	99 [662; Ribose-5-phospha	92	[680; Glycerol-2-phosphate (4TMS)]	39	0.571	0.686	8.173	0.558	20	121	35	106	18	52 duplicate
9042	99 [662; Ribose-5-phospha	101	[832; Dopamine (4TMS)]	41	0.539	0.678	12.485	0.456	21	120	37	104	60	83 original
18619	99 [662; Ribose-5-phospha	91	[766; beta-D-Methylglucopyranoside (4TMS)]	41	0.532	0.684	16.798	0.442	22	119	36	105	88	89 duplicate
16763	99 [662; Ribose-5-phospha	62	[812; D-Xylofuranose (4TMS)]	41	0.515	0.868	11.613	0.647	23	118	17	124	50	15 duplicate
10041	99 [662; Ribose-5-phospha	1	[938; Sulfuric acid (2TMS)]	34	0.512	0.806	4.952	0.616	24	117	23	118	90	25 duplicate
11515	99 [662; Ribose-5-phospha	12	Glyceric acid	40	0.510	0.881	5.476	0.590	25	116	25	116	4	38 duplicate
14518	99 [662; Ribose-5-phospha	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	41	0.488	0.933	11.475	0.555	27	114	8	133	47	47 duplicate
18248	99 [662; Ribose-5-phospha	84	Mannitol	39	0.449	0.633	31.675	0.548	28	113	42	99	131	56 duplicate
18304	99 [662; Ribose-5-phospha	85	[529; Methylcitric acid (4TMS)]	25	0.440	0.788	9.583	0.400	29	112	28	113	29	105 duplicate
18716	99 [662; Ribose-5-phospha	93	[607; Putrescine (4TMS)]	40	0.418	0.433	8.552	0.360	30	111	57	84	20	119 duplicate
9069	99 [662; Ribose-5-phospha	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	36	0.416	0.778	9.737	0.583	31	110	29	112	30	43 original
11770	99 [662; Ribose-5-phospha	14	Fumaric acid	41	0.354	0.865	6.266	0.591	32	109	18	123	8	36 duplicate
9053	99 [662; Ribose-5-phospha	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	41	0.341	0.616	8.767	0.515	33	108	47	94	25	63 original



15943	99 [662; Ribose-5-phosphat	53	Glycerol-2-phosphate	41	0.339	0.367	7.383	0.429	34	107	63	78	13	93 duplicate
18413	99 [662; Ribose-5-phosphat	87	[945; beta-D-Glucopyranose (5TMS)]	39	0.339	0.613	34.466	0.551	35	106	48	93	136	55 duplicate
12750	99 [662; Ribose-5-phosphat	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	35	0.334	0.892	4.086	0.621	36	105	15	128	2	24 duplicate
9061	99 [662; Ribose-5-phosphat	120	[945; Uridine (3TMS)]	39	0.323	0.265	15.180	0.581	37	104	70	71	78	44 original
16841	99 [662; Ribose-5-phosphat	63	Glutamine	39	0.298	-0.344	13.624	0.587	38	103	95	46	66	40 duplicate
9066	99 [662; Ribose-5-phosphat	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	41	0.298	0.635	32.022	0.584	39	102	41	100	132	49 original
18569	99 [662; Ribose-5-phosphat	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	41	0.293	0.392	10.292	0.372	40	101	61	80	40	113 duplicate
12631	99 [662; Ribose-5-phosphat	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	41	0.290	0.631	19.295	0.500	41	100	44	97	100	68 duplicate
17359	99 [662; Ribose-5-phosphat	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	34	0.283	0.362	20.224	0.485	42	99	65	76	103	75 duplicate
15400	99 [662; Ribose-5-phosphat	47	[NA]	41	0.280	0.366	11.290	0.598	43	98	64	77	44	32 duplicate
17566	99 [662; Ribose-5-phosphat	73	[708; Glucose methoxyamine (5TMS)]	34	0.258	0.540	9.858	0.423	44	97	50	91	32	97 duplicate
17891	99 [662; Ribose-5-phosphat	78	Mannose	40	0.254	0.626	8.746	0.553	45	96	46	95	24	54 duplicate
14721	99 [662; Ribose-5-phosphat	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	41	0.244	0.707	33.338	0.584	46	95	31	110	134	42 duplicate
135														
9076	99 [662; Ribose-5-phosphat	102	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	41	0.234	0.493	15.575	0.422	47	94	54	87	83	98 original
9043	99 [662; Ribose-5-phosphat	102	[904; Galactose methoxyamine (5TMS)]	41	0.232	0.586	8.404	0.541	48	93	49	92	19	57 original
13216	99 [662; Ribose-5-phosphat	26	Citramalic acid	41	0.210	0.629	18.872	0.485	49	92	45	96	96	76 duplicate
13443	99 [662; Ribose-5-phosphat	28	Malic acid	41	0.195	0.841	13.108	0.577	50	91	22	119	64	46 duplicate
10726	99 [662; Ribose-5-phosphat	6	Glycerol	41	0.188	0.399	39.525	0.440	51	90	60	81	140	90 duplicate
9047	99 [662; Ribose-5-phosphat	106	[733; Threitol (4TMS)]	40	0.182	0.639	13.140	0.652	52	89	39	102	65	14 original
9041	99 [662; Ribose-5-phosphat	100	[657; Mannitol (6TMS)]	41	0.171	0.701	12.974	0.586	53	88	33	108	63	41 original
9068	99 [662; Ribose-5-phosphat	127	[777; Fructose-6-phosphate methoxyamine (8TMS)]	33	0.155	0.520	5.274	0.604	54	87	51	90	6	30 original
17764	99 [662; Ribose-5-phosphat	35	Fructose	41	0.148	0.703	27.390	0.563	55	86	32	109	121	50 duplicate
14206	99 [662; Ribose-5-phosphat	76	Pyrogutamic acid	41	0.141	0.700	39.353	0.590	56	85	34	107	139	39 duplicate
9057	99 [662; Ribose-5-phosphat	116	[682; Pseudouridine (5TMS)]	22	0.134	0.641	7.084	0.389	57	84	38	103	12	110 original
15855	99 [662; Ribose-5-phosphat	52	[NA]	30	0.117	-0.345	15.209	0.606	58	83	96	45	79	28 duplicate
17498	99 [662; Ribose-5-phosphat	72	[919; D-Xylopyranose (4TMS)]	40	0.105	-0.114	10.089	0.395	59	82	88	53	35	108 duplicate
15565	99 [662; Ribose-5-phosphat	49	[877; Pyrophosphoric acid (4TMS)]	41	0.102	-0.250	16.239	0.486	60	81	92	49	87	73 duplicate
9048	99 [662; Ribose-5-phosphat	107	9-(Z)-Octadecanoic acid	41	0.085	0.080	16.864	0.335	61	80	81	60	89	125 original
9058	99 [662; Ribose-5-phosphat	117	[724; Glycerol (3TMS)]	39	0.082	0.512	9.281	0.561	62	79	53	88	27	51 original
13101	99 [662; Ribose-5-phosphat	25	[709; 2,5-Diaminovalerolactam (2TMS)]	36	0.060	-0.825	15.553	0.627	63	78	133	8	82	23 duplicate
9072	99 [662; Ribose-5-phosphat	131	[626; 5-Methylthioadenosine (3TMS)]	33	0.053	-0.394	11.741	0.443	64	77	99	42	51	88 original
18014	99 [662; Ribose-5-phosphat	80	[772; D-Glucose (5TMS)]	39	0.053	0.460	30.063	0.501	65	76	55	86	127	66 duplicate
9073	99 [662; Ribose-5-phosphat	132	[695; Isomaltose methoxyamine (8TMS)]	33	0.042	0.772	4.239	0.604	66	75	30	111	3	29 original
9051	99 [662; Ribose-5-phosphat	110	[715; Erythritol (4TMS)]	38	0.027	0.516	9.025	0.678	67	74	52	89	26	3 original
9056	99 [662; Ribose-5-phosphat	115	Glucose-6-phosphate	41	0.024	0.632	26.686	0.642	68	72	43	98	117	17 original
12268	99 [662; Ribose-5-phosphat	18	[590; 1-Acetyl-2-thiopyranoside]	41	0.024	0.293	12.130	0.400	69	73	68	73	58	106 duplicate
9063	99 [662; Ribose-5-phosphat	122	[644; Erythritol (4TMS)]	38	0.021	0.636	6.566	0.634	70	71	40	101	9	22 original
9062	99 [662; Ribose-5-phosphat	121	[657; Erythritol (4TMS)]	38	0.010	0.412	7.048	0.513	71	70	58	83	11	65 original
9045	99 [662; Ribose-5-phosphat	104	[795; Erythritol (4TMS)]	40	0.000	0.159	11.421	0.446	72	68	75	66	45	86 original
16884	99 [662; Ribose-5-phosphat	81	[NA]	41	0.000	-0.424	10.772	0.475	73	69	103	38	42	78 duplicate
9060	99 [662; Ribose-5-phosphat	119	[931; myo-Inositol-2-phosphate (7TMS)]	41	-0.007	0.121	11.495	0.391	74	67	77	64	49	109 original
16918	99 [662; Ribose-5-phosphat	64	[789; Tyramine (3TMS)]	41	-0.022	0.047	8.290	0.404	75	66	82	59	28	104 duplicate
9052	99 [662; Ribose-5-phosphat	111	[583; Erythritol (4TMS)]	32	-0.024	0.197	12.652	0.329	76	65	72	69	62	126 original
17633	99 [662; Ribose-5-phosphat	74	[912; Tetradecanoic acid (1TMS)]	41	-0.039	0.328	11.780	0.497	77	64	66	75	54	70 duplicate
9067	99 [662; Ribose-5-phosphat	126	[559; Erythritol (4TMS)]	36	-0.048	0.253	8.154	0.596	78	63	71	70	17	34 original
11896	99 [662; Ribose-5-phosphat	15	Alanine	41	-0.061	-0.009	18.987	0.540	79	62	83	58	102	58 duplicate
9054	99 [662; Ribose-5-phosphat	113	Galactose-6-phosphate	41	-0.071	0.447	8.559	0.570	80	60	56	85	21	48 original
12380	99 [662; Ribose-5-phosphat	19	Alanine (BP) (3TMS)	41	-0.071	0.325	15.458	0.499	81	61	67	74	81	69 duplicate
18518	99 [662; Ribose-5-phosphat	89	[775; Dopamine (4TMS)]	21	-0.076	-0.622	14.333	0.369	82	59	114	27	71	115 duplicate
9050	99 [662; Ribose-5-phosphat	109	Octadecanoic acid	41	-0.105	0.083	26.011	0.460	83	58	80	61	116	82 original

15018	99 [662; Ribose-5-phospha	43	[548; Leucine (2TBS)]	37	-0.111	-0.361	12.016	0.404	84	57	97	44	56	103 duplicate
15115	99 [662; Ribose-5-phospha	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	36	-0.121	0.381	11.765	0.591	85	58	62	79	52	35 duplicate
18763	99 [662; Ribose-5-phospha	94	Hexadecanoic acid	41	-0.122	0.087	24.216	0.462	86	55	79	82	114	81 duplicate
90555	99 [662; Ribose-5-phospha	114	Fructose-6-phosphate	40	-0.126	0.399	7.608	0.557	87	54	59	82	14	53 original
9074	99 [662; Ribose-5-phospha	133	[855; Squalene]	41	-0.129	-0.068	11.999	0.424	88	53	87	54	55	96 original
9082	99 [662; Ribose-5-phospha	141	Lanosta-8,24-dien-3-beta-ol	38	-0.132	0.111	8.595	0.480	89	52	78	63	22	77 original
9080	99 [662; Ribose-5-phospha	139	[700; Ergosta-5,7-dien-3-ol]	28	-0.133	-0.056	11.460	0.338	90	51	88	55	46	123 original
9081	99 [662; Ribose-5-phospha	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	32	-0.133	0.178	8.046	0.451	91	50	73	68	15	85 original
18854	99 [662; Ribose-5-phospha	96	myo-Inositol	31	-0.140	-0.031	10.104	0.220	92	49	84	57	36	138 duplicate
14921	99 [662; Ribose-5-phospha	41	[639; Proline (2TMS)]	41	-0.141	0.169	17.046	0.446	93	48	74	67	91	87 duplicate
9071	99 [662; Ribose-5-phospha	130	Trehalose	41	-0.156	-0.145	28.601	0.439	94	47	89	52	125	91 original
18809	99 [662; Ribose-5-phospha	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	27	-0.157	-0.419	13.801	0.308	95	46	102	39	68	132 duplicate
17953	99 [662; Ribose-5-phospha	79	Glucose	41	-0.161	0.271	33.618	0.527	96	45	69	72	135	60 duplicate
9064	99 [662; Ribose-5-phospha	123	[945; Galactoturanose-6-phosphate (7TMS)]	41	-0.173	0.155	14.377	0.519	97	44	76	65	72	61 original
12511	99 [662; Ribose-5-phospha	20	[919; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	14	-0.187	-0.676	10.027	0.434	98	43	119	22	34	92 duplicate
8049	99 [662; Ribose-5-phospha	108	Octadecanoic acid	41	-0.202	-0.328	9.945	0.368	99	42	94	47	33	116 original
9065	99 [662; Ribose-5-phospha	124	[734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]	39	-0.215	-0.253	15.100	0.473	100	41	93	48	77	79 original
15493	99 [662; Ribose-5-phospha	48	Asparagine	41	-0.217	-0.741	14.632	0.613	101	40	128	15	73	26 duplicate
18191	99 [662; Ribose-5-phospha	83	Sorbitol	35	-0.230	-0.410	22.938	0.293	102	39	101	40	112	135 duplicate
18941	99 [662; Ribose-5-phospha	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	27	-0.231	-0.708	15.581	0.367	103	38	124	17	84	117 duplicate
9078	99 [662; Ribose-5-phospha	137	Ergosterol	41	-0.239	-0.161	17.897	0.377	104	37	90	51	93	111 original
12868	99 [662; Ribose-5-phospha	23	Homoserine	41	-0.244	-0.791	14.207	0.497	105	36	131	10	70	71 duplicate
15211	99 [662; Ribose-5-phospha	45	Homocysteine	38	-0.249	-0.498	15.029	0.413	106	35	104	37	76	101 duplicate
9077	99 [662; Ribose-5-phospha	138	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.250	-0.406	5.062	0.335	107	34	100	41	5	124 original
9059	99 [662; Ribose-5-phospha	118	[928; Glucopyranose-6-phosphate (6TMS)]	40	-0.264	-0.045	10.438	0.486	108	33	85	56	39	74 original
9079	99 [662; Ribose-5-phospha	138	[674; Ergosterol (1TMS)]	34	-0.298	-0.169	10.707	0.397	109	32	91	50	41	107 original
17216	99 [662; Ribose-5-phospha	68	[570; Hypoxanthine (2TMS)]	12	-0.333	-0.945	11.274	0.228	110	31	136	5	43	137 duplicate
17429	99 [662; Ribose-5-phospha	71	[731; Erythrose (3TMS)]	41	-0.334	-0.362	15.724	0.422	111	30	98	43	86	99 duplicate
14100	99 [662; Ribose-5-phospha	34	Aspartic acid	41	-0.385	-0.528	30.389	0.326	112	29	107	34	128	127 duplicate
11256	99 [662; Ribose-5-phospha	10	Glycine	41	-0.388	-0.853	19.851	0.612	113	28	138	3	101	27 duplicate
10455	99 [662; Ribose-5-phospha	4	Phosphoric acid	29	-0.429	-0.515	31.306	0.191	114	27	105	36	130	139 duplicate
14311	99 [662; Ribose-5-phospha	36	[596; N-Acetylglutamic acid (2TMS)]	41	-0.441	-0.596	27.717	0.355	115	25	111	30	123	121 duplicate
13993	99 [662; Ribose-5-phospha	33	Methionine	41	-0.441	-0.619	14.767	0.311	116	26	113	28	75	131 duplicate
16804	99 [662; Ribose-5-phospha	60	Glycerol-3-phosphate	41	-0.446	-0.595	22.812	0.492	117	24	110	31	110	72 duplicate
17899	99 [662; Ribose-5-phospha	75	Lysine	41	-0.451	-0.626	36.221	0.345	118	23	115	26	137	122 duplicate
13330	99 [662; Ribose-5-phospha	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	30	-0.457	-0.839	18.506	0.428	119	22	135	6	94	95 duplicate
16441	99 [662; Ribose-5-phospha	58	[636; 4R-Acetamidido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	41	-0.459	-0.523	18.644	0.361	120	21	106	35	95	118 duplicate
17288	99 [662; Ribose-5-phospha	59	Arginine	37	-0.465	-0.878	21.224	0.591	121	20	139	2	108	45 duplicate
16116	99 [662; Ribose-5-phospha	55	[612; 4-Aminobutyric acid (2TBS)]	21	-0.467	-0.671	12.586	0.377	122	19	117	24	61	112 duplicate
17143	99 [662; Ribose-5-phospha	67	Citric acid	41	-0.468	-0.557	24.398	0.371	123	17	108	33	115	114 duplicate
13776	99 [662; Ribose-5-phospha	31	[622; Parabenic acid (2TMS)]	41	-0.468	-0.737	11.479	0.465	124	18	125	16	48	80 duplicate
15766	99 [662; Ribose-5-phospha	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	23	-0.470	-0.788	13.773	0.311	125	16	130	11	67	130 duplicate
13668	99 [662; Ribose-5-phospha	30	[815; Ethyl-3-(2H)-thiophenone]	41	-0.476	-0.640	27.817	0.323	126	15	116	25	124	128 duplicate
14415	99 [662; Ribose-5-phospha	37	Phenylalanine	41	-0.502	-0.674	23.546	0.451	127	14	118	23	113	84 duplicate
10318	99 [662; Ribose-5-phospha	3	Ethanolamine	39	-0.514	-0.746	12.083	0.514	128	13	127	14	57	64 duplicate
10860	99 [662; Ribose-5-phospha	7	Threonine	41	-0.529	-0.596	29.316	0.272	129	12	112	29	126	136 duplicate
18133	99 [662; Ribose-5-phospha	82	Lysine	21	-0.533	-0.908	15.708	0.501	130	11	140	1	85	67 duplicate
17069	99 [662; Ribose-5-phospha	66	Glycemic acid-3-phosphate	41	-0.534	-0.707	10.322	0.428	131	10	123	18	38	94 duplicate

16523	99 [662; Ribose-5-phosphat	59	Omitrine; Arginine	41	-0.541	-0.690	38,951	0.411	132	9	121	20	138	102 duplicate
10993	99 [662; Ribose-5-phosphat	8	Isoleucine	32	-0.569	-0.577	21,016	0.186	133	8	109	32	106	140 duplicate
10591	99 [662; Ribose-5-phosphat	5	Leucine	22	-0.576	-0.822	11,780	0.323	134	7	132	9	53	129 duplicate
14920	99 [662; Ribose-5-phosphat	42	Glutamic acid	37	-0.589	-0.781	26,882	0.359	135	6	129	12	118	120 duplicate
18074	99 [662; Ribose-5-phosphat	81	Tyrosine	41	-0.590	-0.835	30,819	0.596	136	5	134	7	129	33 duplicate
11125	99 [662; Ribose-5-phosphat	9	Proline	40	-0.595	-0.692	26,899	0.298	137	4	122	19	119	134 duplicate
17828	99 [662; Ribose-5-phosphat	77	benzeneacetic acid methyl ester	39	-0.598	-0.766	27,709	0.418	138	3	128	13	122	100 duplicate
13885	99 [662; Ribose-5-phosphat	32	[728; N,N-Dimethyllysine methyl ester]	40	-0.603	-0.850	17,799	0.529	139	2	137	4	92	59 duplicate
10180	99 [662; Ribose-5-phosphat	2	Serine	39	-0.692	-0.679	21,218	0.306	140	1	120	21	107	133 duplicate
9084	100 [857; Mannitol (6TMS)]	102	[904; Galactose methoxyamine (5TMS)]	64	0.752	0.926	7,760	0.619	1	141	1	141	25	1 original
9097	100 [857; Mannitol (6TMS)]	115	Glucose-6-phosphate	62	0.692	0.681	17,768	0.584	2	140	38	104	83	8 original
13444	100 [857; Mannitol (6TMS)]	28	Malic acid	64	0.672	0.857	2,023	0.560	3	139	2	140	1	15 duplicate
9094	100 [857; Mannitol (6TMS)]	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.662	0.831	19,529	0.560	4	138	6	136	105	16 original
9108	100 [857; Mannitol (6TMS)]	126	[558; Erythritol (4TMS)]	45	0.648	0.769	9,446	0.597	5	137	17	125	34	3 original
9117	100 [857; Mannitol (6TMS)]		[902; Melibiose (6TMS); alpha-D-Gal-(1,6)-D-Glc (6TMS)]	64	0.642	0.801	5,059	0.533	6	136	8	134	7	39 original
14207	100 [857; Mannitol (6TMS)]	35	Pyrogalluric acid	64	0.618	0.656	34,665	0.540	7	135	44	98	139	36 duplicate
15116	100 [857; Mannitol (6TMS)]	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	0.613	0.785	7,559	0.530	8	134	10	132	20	40 duplicate
9099	100 [857; Mannitol (6TMS)]	117	[724; Glycerol (3TMS)]	56	0.609	0.773	9,398	0.571	9	133	16	126	30	9 original
14722	100 [857; Mannitol (6TMS)]	40	[880; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.608	0.783	27,836	0.525	10	132	13	129	132	45 duplicate
9104	100 [857; Mannitol (6TMS)]	122	[644; Erythritol (4TMS)]	52	0.597	0.775	17,454	0.559	11	131	15	127	92	18 original
9103	100 [857; Mannitol (6TMS)]	121	[657; Erythritol (4TMS)]	55	0.595	0.695	16,410	0.524	12	130	33	109	85	47 original
11516	100 [857; Mannitol (6TMS)]	12	Glyceric acid	63	0.586	0.832	13,293	0.561	13	129	4	138	67	14 duplicate
17765	100 [857; Mannitol (6TMS)]	76	Fructose	64	0.582	0.640	19,062	0.508	14	128	47	95	102	50 duplicate
9092	100 [857; Mannitol (6TMS)]	110	[715; Erythritol (4TMS)]	54	0.574	0.670	13,169	0.576	15	127	41	101	65	7 original
9088	100 [857; Mannitol (6TMS)]	106	[733; Threitol (4TMS)]	62	0.562	0.706	8,154	0.541	16	126	28	114	27	35 original
11771	100 [857; Mannitol (6TMS)]	14	Fumaric acid	64	0.559	0.791	11,196	0.529	17	125	11	131	49	41 duplicate
17634	100 [857; Mannitol (6TMS)]	74	[912; Tetradecanoic acid (1TMS)]	64	0.557	0.687	10,284	0.467	18	124	38	106	40	64 duplicate
9096	100 [857; Mannitol (6TMS)]	114	Fructose-6-phosphate	53	0.554	0.675	11,049	0.504	19	123	39	103	46	51 original
14519	100 [857; Mannitol (6TMS)]	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.552	0.840	3,201	0.557	20	122	3	139	3	21 duplicate
12751	100 [857; Mannitol (6TMS)]	22	[690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.549	0.788	14,302	0.556	21	121	12	130	73	22 duplicate
9098	100 [857; Mannitol (6TMS)]	116	[882; Pseudouridine (5TMS)]	30	0.545	0.664	9,430	0.409	22	120	42	100	33	104 original
13556	100 [857; Mannitol (6TMS)]	29	Erythritol	64	0.528	0.816	5,953	0.554	23	118	7	135	11	26 duplicate
12632	100 [857; Mannitol (6TMS)]	21	[678; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	64	0.528	0.686	9,399	0.495	24	119	37	105	31	57 duplicate
18305	100 [857; Mannitol (6TMS)]	85	[529; Methylcitric acid (4TMS)]	48	0.516	0.747	4,454	0.460	26	116	22	120	5	67 duplicate
9114	100 [857; Mannitol (6TMS)]	132	[895; Isomaltose methoxyamine (6TMS)]	42	0.515	0.832	17,243	0.564	27	115	5	137	80	12 original
11387	100 [857; Mannitol (6TMS)]	11	Succinic acid	64	0.513	0.754	2,974	0.504	28	114	21	121	2	52 duplicate
16764	100 [857; Mannitol (6TMS)]	62	[812; D-Xylofuranose (4TMS)]	64	0.508	0.701	6,858	0.537	29	113	30	112	17	37 duplicate
9095	100 [857; Mannitol (6TMS)]	113	Galactose-6-phosphate	62	0.498	0.579	10,466	0.442	30	112	53	89	43	81 original
17892	100 [857; Mannitol (6TMS)]	78	Mannose	62	0.481	0.648	12,238	0.486	31	111	45	97	58	60 duplicate
12269	100 [857; Mannitol (6TMS)]	18	[590; 1-Acetyl-2-thiohydantoin]	64	0.478	0.568	3,784	0.431	32	110	54	88	4	89 duplicate
13217	100 [857; Mannitol (6TMS)]	26	Citramalic acid	64	0.475	0.642	9,332	0.486	33	109	46	96	29	59 duplicate
14621	100 [857; Mannitol (6TMS)]	39	[829; 1-Phenylethanol (1TMS)]	63	0.471	0.797	11,123	0.551	34	108	9	133	47	28 duplicate
18360	100 [857; Mannitol (6TMS)]	86	[793; D-Galactono-1,4-lactone (4TMS)]	61	0.458	0.663	18,104	0.555	35	107	43	99	94	24 duplicate
17360	100 [857; Mannitol (6TMS)]	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	0.457	0.775	12,334	0.341	36	106	60	82	59	133 duplicate
12022	100 [857; Mannitol (6TMS)]	14	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	0.457	0.477	10,642	0.558	37	104	14	128	44	19 duplicate
12886	100 [857; Mannitol (6TMS)]	24	[725; 2-Ketobutanolic acid (2TMS)]	64	0.457	0.761	25,223	0.553	38	105	19	123	125	27 duplicate
16031	100 [857; Mannitol (6TMS)]	54	[NA]	55	0.455	0.761	13,560	0.528	39	103	18	124	69	43 duplicate
16275	100 [857; Mannitol (6TMS)]	56	[829; Orotic acid (3TMS)]	64	0.454	0.712	12,238	0.544	40	102	27	115	57	31 duplicate
9109	100 [857; Mannitol (6TMS)]	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.449	0.631	6,507	0.587	41	101	48	94	14	4 original

18669	100 [857; Mannitol (6TMS)]	92 [680; Glycerol-2-phosphate (4TMS)]	54 0.434	0.478	9.428	0.460	42	100	59	83	32	68 duplicate
9102	100 [857; Mannitol (6TMS)]	120 [945; Uridine (3TMS)]	54 0.433	0.278	6.166	0.567	43	99	74	68	13	11 original
17567	100 [857; Mannitol (6TMS)]	73 [708; Glucose methoxyamine (5TMS)]	57 0.424	0.623	11.174	0.423	44	98	50	92	48	95 duplicate
15307	100 [857; Mannitol (6TMS)]	46 Arabinose	64 0.423	0.703	13.543	0.529	45	97	29	113	68	42 duplicate
9116	100 [857; Mannitol (6TMS)]	134 Isomaltose	64 0.422	0.724	18.939	0.548	46	96	25	117	100	29 original
9107	100 [857; Mannitol (6TMS)]	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64 0.415	0.481	25.522	0.452	47	95	57	85	127	75 original
9110	100 [857; Mannitol (6TMS)]	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45 0.414	0.760	5.527	0.563	48	94	20	122	9	13 original
18467	100 [857; Mannitol (6TMS)]	88 Gluconic acid	64 0.413	0.688	7.607	0.554	49	93	35	107	21	25 duplicate
16995	100 [857; Mannitol (6TMS)]	65 [646; 3-Deoxyglucitol (5TMS)]	63 0.408	0.747	14.141	0.570	50	92	23	119	71	10 duplicate
15677	100 [857; Mannitol (6TMS)]	57 [746; Ribonic acid-1,4-lactone (3TMS)]	61 0.402	0.693	21.536	0.547	51	91	34	108	108	30 duplicate
12146	100 [857; Mannitol (6TMS)]	17 [700; 2-methyl-1,2-propanediol (2TMS)]	64 0.401	0.722	10.778	0.497	52	90	26	116	45	55 duplicate
9111	100 [857; Mannitol (6TMS)]	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59 0.398	0.697	11.446	0.576	53	89	32	110	50	8 original
18359	100 [857; Mannitol (6TMS)]	57 [757; 2-Deoxy-pentose-3-yose dimethoxyamine (2TMS)]	55 0.389	0.673	11.669	0.543	54	88	40	102	51	32 duplicate
11644	100 [857; Mannitol (6TMS)]	13 Uracil	64 0.372	0.730	9.759	0.558	55	87	24	118	38	20 duplicate
9085	100 [857; Mannitol (6TMS)]	103 [648; Ethylamine (2TMS)]	63 0.368	0.587	11.855	0.464	56	86	52	90	52	65 original
18192	100 [857; Mannitol (6TMS)]	83 Sorbitol	58 0.360	-0.048	15.758	0.321	57	85	88	54	79	139 duplicate
18855	100 [857; Mannitol (6TMS)]	96 myo-inositol	49 0.342	0.316	22.040	0.353	58	84	70	72	113	131 duplicate
9091	100 [857; Mannitol (6TMS)]	109 Octadecanoic acid	64 0.339	0.535	16.443	0.425	59	83	56	86	86	94 original
9093	100 [857; Mannitol (6TMS)]	111 [583; Erythritol (4TMS)]	42 0.333	0.559	22.745	0.499	60	82	55	87	115	53 original
9122	100 [857; Mannitol (6TMS)]	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49 0.327	0.344	18.264	0.395	61	81	68	74	96	108 original
9087	100 [857; Mannitol (6TMS)]	105 [705; 2-Ketogluconic acid (5TMS)]	48 0.316	0.626	9.447	0.498	62	80	49	93	35	54 original
18764	100 [857; Mannitol (6TMS)]	94 Hexadecanoic acid	64 0.303	0.481	15.110	0.412	63	79	58	84	76	102 duplicate
9105	100 [857; Mannitol (6TMS)]	123 [945; Galactofuranose-6-phosphate (7TMS)]	64 0.294	0.293	5.173	0.431	65	77	65	77	15	88 duplicate
12391	100 [857; Mannitol (6TMS)]	19 Alanine (BP) (3TMS)	64 0.292	0.360	6.813	0.391	66	76	63	79	82	110 original
9123	100 [857; Mannitol (6TMS)]	141 Lanosta-8,24-dien-3-beta-ol	61 0.289	0.384	16.234	0.382	67	75	73	69	101	71 original
9120	100 [857; Mannitol (6TMS)]	138 [674; Ergosterol (1TMS)]	46 0.266	0.282	18.969	0.457	67	75	61	81	36	112 original
9086	100 [857; Mannitol (6TMS)]	101 [832; Dopamine (4TMS)]	64 0.263	0.452	9.464	0.389	68	74	61	81	36	112 original
9083	100 [857; Mannitol (6TMS)]	104 [795; Erythritol (4TMS)]	63 0.259	0.342	7.716	0.370	69	73	69	73	23	124 original
17430	100 [857; Mannitol (6TMS)]	71 [731; Erythrose (3TMS)]	64 0.239	0.172	5.731	0.437	70	72	79	63	10	84 duplicate
10727	100 [857; Mannitol (6TMS)]	6 Glycerol	64 0.238	0.355	35.302	0.378	71	71	68	76	141	119 duplicate
18899	100 [857; Mannitol (6TMS)]	97 [756; beta-D-Methylglucopyranoside (4TMS)]	52 0.223	0.400	16.800	0.441	72	70	62	80	88	82 duplicate
14822	100 [857; Mannitol (6TMS)]	41 [639; Proline (2TMS)]	64 0.223	0.230	7.729	0.410	73	69	77	65	24	103 duplicate
9115	100 [857; Mannitol (6TMS)]	133 [855; Squalene]	84 0.214	0.135	7.618	0.380	74	68	81	61	22	115 original
18820	100 [857; Mannitol (6TMS)]	91 [766; beta-D-Methylglucopyranoside (4TMS)]	64 0.213	0.383	15.921	0.414	75	67	64	78	80	101 duplicate
9119	100 [857; Mannitol (6TMS)]	137 Ergosterol	64 0.184	0.079	10.385	0.361	76	66	84	58	42	128 original
18249	100 [857; Mannitol (6TMS)]	84 Mannitol	62 0.176	0.354	25.585	0.419	77	65	67	75	128	88 duplicate
18984	100 [857; Mannitol (6TMS)]	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41 0.171	0.701	12.974	0.586	78	64	31	111	64	5 duplicate
16919	100 [857; Mannitol (6TMS)]	64 [789; Tyramine (3TMS)]	63 0.156	0.226	7.181	0.382	79	63	78	64	19	114 duplicate
18414	100 [857; Mannitol (6TMS)]	97 [945; beta-D-Glucopyranose (5TMS)]	62 0.120	0.266	29.294	0.432	80	62	75	67	137	87 duplicate
18717	100 [857; Mannitol (6TMS)]	93 [607; Putrescine (4TMS)]	60 0.116	0.301	19.297	0.373	81	61	71	71	103	123 duplicate
17954	100 [857; Mannitol (6TMS)]	78 Glucose	64 0.093	0.242	26.608	0.446	82	60	76	68	135	78 duplicate
11897	100 [857; Mannitol (6TMS)]	15 Alanine	64 0.082	0.036	12.827	0.496	83	59	87	55	62	56 duplicate
9121	100 [857; Mannitol (6TMS)]	139 [700; Ergosta-5,7-dien-3-ol]	38 0.075	-0.083	20.776	0.388	84	58	90	52	107	113 original
9101	100 [857; Mannitol (6TMS)]	119 [831; myo-Inositol-2-phosphate (7TMS)]	64 0.065	0.154	7.145	0.365	85	57	80	62	18	126 original
18015	100 [857; Mannitol (6TMS)]	80 [772; D-Glucose (5TMS)]	62 0.052	0.133	25.016	0.378	86	56	82	60	124	116 duplicate
9106	100 [857; Mannitol (6TMS)]	124 [734; 1-Monoolcylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	59 0.045	-0.119	26.611	0.391	87	55	92	50	130	111 original
9118	100 [857; Mannitol (6TMS)]	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17 0.029	0.088	4.841	0.559	88	54	83	59	6	17 original
18570	100 [857; Mannitol (6TMS)]	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	64 -0.016	0.037	6.141	0.327	89	52	86	56	12	138 duplicate

9089	100 [857; Mannitol (6TMS)]	107 9-(Z)-Octadecenoic acid	64 -0.016	-0.090	8.579	0.338	90	53	91	51	28	135 original
9100	100 [857; Mannitol (6TMS)]	118 [928; Glucopyranose-6-phosphate (6TMS)]	58 -0.051	-0.215	12.030	0.455	91	51	98	46	64	73 original
17144	100 [857; Mannitol (6TMS)]	67 Citric acid	64 -0.056	-0.162	17.318	0.334	92	50	83	49	91	136 duplicate
10861	100 [857; Mannitol (6TMS)]	7 Threonine	64 -0.076	-0.304	23.889	0.354	93	49	98	44	119	130 duplicate
16605	100 [857; Mannitol (6TMS)]	60 Glycerol-3-phosphate	64 -0.083	-0.181	15.267	0.378	94	48	95	47	77	122 duplicate
15944	100 [857; Mannitol (6TMS)]	53 Glycerol-2-phosphate	64 -0.105	-0.166	13.959	0.333	95	46	94	48	70	137 duplicate
15401	100 [857; Mannitol (6TMS)]	47 [NA]	64 -0.105	-0.240	12.206	0.450	96	47	97	45	56	76 duplicate
14416	100 [857; Mannitol (6TMS)]	37 Phenylethanol	64 -0.122	-0.309	16.466	0.392	97	45	99	43	87	109 duplicate
10042	100 [857; Mannitol (6TMS)]	1 [938; Sulfuric acid (2TMS)]	36 -0.168	0.051	10.263	0.600	98	44	85	57	39	2 duplicate
15856	100 [857; Mannitol (6TMS)]	52 [NA]	46 -0.181	-0.336	22.096	0.447	99	43	104	38	114	77 duplicate
14312	100 [857; Mannitol (6TMS)]	38 [596; N-Acetylglutamic acid (2TMS)]	64 -0.184	-0.366	22.862	0.396	100	42	106	36	118	107 duplicate
16117	100 [857; Mannitol (6TMS)]	55 [612; 4-Aminobutyric acid (2TBS)]	43 -0.192	-0.318	23.743	0.361	101	41	101	41	118	127 duplicate
10994	100 [857; Mannitol (6TMS)]	8 Isoleucine	55 -0.208	-0.331	16.065	0.338	102	40	103	39	81	134 duplicate
9090	100 [857; Mannitol (6TMS)]	108 Octadecenoic acid	64 -0.209	-0.336	10.378	0.377	103	39	105	37	41	121 original
16685	100 [857; Mannitol (6TMS)]	61 [NA]	64 -0.210	-0.051	6.832	0.416	104	38	89	53	16	100 duplicate
10319	100 [857; Mannitol (6TMS)]	3 Ethanolamine	62 -0.217	-0.447	14.575	0.418	105	37	113	29	74	99 duplicate
18810	100 [857; Mannitol (6TMS)]	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50 -0.221	-0.324	21.715	0.318	106	38	102	40	109	140 duplicate
15767	100 [857; Mannitol (6TMS)]	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44 -0.228	-0.558	22.004	0.443	107	35	129	13	112	80 duplicate
17070	100 [857; Mannitol (6TMS)]	66 Glyceric acid-3-phosphate	64 -0.246	-0.399	9.508	0.444	108	34	108	34	37	79 duplicate
12512	100 [857; Mannitol (6TMS)]	20 [619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31 -0.247	-0.429	16.292	0.484	109	33	111	31	83	66 duplicate
9112	100 [857; Mannitol (6TMS)]	130 Trehalose	63 -0.260	-0.422	23.620	0.423	110	31	110	32	117	96 original
17499	100 [857; Mannitol (6TMS)]	72 [919; D-Xylopyranose (4TMS)]	63 -0.260	-0.468	12.464	0.377	111	32	117	25	61	120 duplicate
17829	100 [857; Mannitol (6TMS)]	77 benzeneacetic acid methyl ester	62 -0.276	-0.487	25.359	0.438	112	30	118	24	126	83 duplicate
17700	100 [857; Mannitol (6TMS)]	75 Lysine	64 -0.284	-0.421	33.624	0.357	113	29	109	33	138	128 duplicate
16442	100 [857; Mannitol (6TMS)]	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64 -0.287	-0.383	11.859	0.351	114	28	107	35	53	132 duplicate
11126	100 [857; Mannitol (6TMS)]	9 Proline	63 -0.294	-0.463	24.006	0.378	115	27	116	28	121	118 duplicate
17217	100 [857; Mannitol (6TMS)]	68 [570; Hypoxanthine (2TMS)]	50 -0.295	-0.673	16.357	0.458	116	26	135	7	84	70 duplicate
10456	100 [857; Mannitol (6TMS)]	4 Phosphoric acid	51 -0.296	-0.310	28.073	0.305	117	25	100	42	134	141 duplicate
18075	100 [857; Mannitol (6TMS)]	81 Tyrosine	64 -0.299	-0.510	28.782	0.453	118	24	121	21	136	74 duplicate
14101	100 [857; Mannitol (6TMS)]	34 Aspartic acid	64 -0.311	-0.458	27.083	0.436	119	23	115	27	131	85 duplicate
15212	100 [857; Mannitol (6TMS)]	45 Homocysteine	61 -0.311	-0.454	24.788	0.421	120	22	114	28	122	97 duplicate
10592	100 [857; Mannitol (6TMS)]	5 Leucine	45 -0.321	-0.665	12.852	0.474	121	21	134	8	63	61 duplicate
13667	100 [857; Mannitol (6TMS)]	30 [815; Ethyl-3(2H)-thiophenone]	64 -0.321	-0.529	24.921	0.378	122	20	125	17	123	117 duplicate
18519	100 [857; Mannitol (6TMS)]	89 [775; Dopamine (4TMS)]	35 -0.334	-0.520	18.347	0.402	123	19	124	18	97	105 duplicate
13777	100 [857; Mannitol (6TMS)]	31 [622; Parabanic acid (2TMS)]	64 -0.337	-0.535	14.263	0.468	124	18	126	16	72	63 duplicate
13994	100 [857; Mannitol (6TMS)]	33 Methionine	64 -0.339	-0.543	12.081	0.457	125	16	127	15	55	72 duplicate
15494	100 [857; Mannitol (6TMS)]	48 Asparagine	64 -0.339	-0.548	13.258	0.513	126	17	128	14	68	48 duplicate
10181	100 [857; Mannitol (6TMS)]	2 Serine	62 -0.340	-0.433	16.885	0.365	127	15	112	30	89	125 duplicate
16524	100 [857; Mannitol (6TMS)]	59 Ornithine; Arginine	64 -0.361	-0.508	34.948	0.426	128	14	120	22	140	92 duplicate
17289	100 [857; Mannitol (6TMS)]	69 Arginine	60 -0.365	-0.689	18.139	0.541	129	13	137	5	95	34 duplicate
11257	100 [857; Mannitol (6TMS)]	10 Glycine	64 -0.369	-0.662	14.837	0.542	130	12	133	9	75	33 duplicate
13986	100 [857; Mannitol (6TMS)]	32 [729; N,N-Dimethyllysine methyl ester]	60 -0.396	-0.644	19.728	0.535	131	11	132	10	108	38 duplicate
14921	100 [857; Mannitol (6TMS)]	42 Glutamic acid	60 -0.398	-0.602	26.265	0.433	132	10	131	11	129	86 duplicate
16942	100 [857; Mannitol (6TMS)]	63 Glutamine	52 -0.403	-0.497	18.525	0.528	133	9	119	23	98	44 duplicate
12869	100 [857; Mannitol (6TMS)]	23 Homoserine	64 -0.406	-0.739	12.404	0.525	134	8	139	3	60	46 duplicate
18134	100 [857; Mannitol (6TMS)]	82 Lysine	39 -0.414	-0.721	15.652	0.495	135	7	138	4	78	58 duplicate
13331	100 [857; Mannitol (6TMS)]	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53 -0.422	-0.686	21.742	0.472	136	6	136	6	110	62 duplicate
15586	100 [857; Mannitol (6TMS)]	49 [877; Pyrophosphoric acid (4TMS)]	64 -0.436	-0.516	23.965	0.426	137	5	122	20	120	93 duplicate

15019	100 [857; Mannitol (6TMS)]	43	[548; Leucine (2TBS)]	60	-0.436	-0.520	7.851	0.398	138	4	123	19	26	106 duplicate
18942	100 [857; Mannitol (6TMS)]	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	48	-0.454	-0.747	21.872	0.512	139	3	140	2	111	49 duplicate
9113	100 [857; Mannitol (6TMS)]	131	[626; 5-Methylthioadenosine (3TMS)]	55	-0.468	-0.586	19.481	0.427	140	2	130	12	104	90 original
13102	100 [857; Mannitol (6TMS)]	25	[708; 2,5-Diaminovalerolactam (2TMS)]	48	-0.568	-0.790	18.873	0.556	141	1	141	1	99	23 duplicate
9125	101 [832; Dopamine (4TMS)]	103	[648; Ethylamine (2TMS)]	63	0.808	0.958	5.254	0.850	1	141	1	141	1	2 original
18900	101 [832; Dopamine (4TMS)]	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	0.765	0.897	12.634	0.558	2	140	3	139	47	12 duplicate
18621	101 [832; Dopamine (4TMS)]	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	0.694	0.824	8.555	0.827	3	139	2	140	8	4 duplicate
9127	101 [832; Dopamine (4TMS)]	105	[705; 2-Ketogluconic acid (5TMS)]	48	0.674	0.873	5.594	0.587	4	138	4	138	2	8 original
18670	101 [832; Dopamine (4TMS)]	92	[680; Glyceral-2-phosphate (4TMS)]	54	0.616	0.635	8.800	0.395	5	137	26	116	11	110 duplicate
9156	101 [832; Dopamine (4TMS)]	134	Isomaltose	64	0.581	0.757	19.615	0.534	6	136	6	136	91	21 original
16276	101 [832; Dopamine (4TMS)]	56	[829; Orotic acid (3TMS)]	64	0.572	0.754	9.485	0.542	7	135	8	134	17	17 duplicate
16986	101 [832; Dopamine (4TMS)]	65	[646; 3-Deoxyglucitol (5TMS)]	63	0.563	0.722	11.209	0.526	8	134	14	128	27	26 duplicate
15308	101 [832; Dopamine (4TMS)]	46	Arabinose	64	0.557	0.743	12.059	0.533	9	133	10	132	43	23 duplicate
18468	101 [832; Dopamine (4TMS)]	88	Gluconic acid	64	0.555	0.690	8.598	0.539	10	132	19	123	9	19 duplicate
11645	101 [832; Dopamine (4TMS)]	13	Uracil	64	0.552	0.768	11.662	0.558	11	131	5	137	36	11 duplicate
9151	101 [832; Dopamine (4TMS)]	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	0.550	0.721	9.058	0.491	12	130	15	127	14	45 original
12023	101 [832; Dopamine (4TMS)]	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	0.550	0.757	14.033	0.562	13	129	7	135	62	10 duplicate
18985	101 [832; Dopamine (4TMS)]	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	0.539	0.678	12.485	0.456	14	128	20	122	46	71 duplicate
12987	101 [832; Dopamine (4TMS)]	24	[725; 2-Ketotartaric acid (2TMS)]	64	0.534	0.751	27.964	0.552	15	127	9	133	123	15 duplicate
12147	101 [832; Dopamine (4TMS)]	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	0.529	0.730	13.543	0.505	16	126	11	131	57	34 duplicate
14622	101 [832; Dopamine (4TMS)]	29	[829; 1-Phenylethanol (1TMS)]	63	0.506	0.707	11.368	0.482	17	125	18	128	30	55 duplicate
13557	101 [832; Dopamine (4TMS)]	28	Erythritol	64	0.495	0.725	8.750	0.509	18	124	12	130	10	30 duplicate
15678	101 [832; Dopamine (4TMS)]	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	0.489	0.724	20.177	0.498	19	123	13	129	94	38 duplicate
16360	101 [832; Dopamine (4TMS)]	57	[757; 2-Deoxy-pentose-3-yose dimethoxyamine (2TMS)]	55	0.487	0.649	10.406	0.460	20	122	23	119	21	67 duplicate
18361	101 [832; Dopamine (4TMS)]	86	[793; D-Galactono-1,4-lactone (4TMS)]	81	0.484	0.694	17.269	0.531	21	121	18	124	80	24 duplicate
14520	101 [832; Dopamine (4TMS)]	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.475	0.696	7.676	0.482	22	120	17	125	6	54 duplicate
18415	101 [832; Dopamine (4TMS)]	87	[945; beta-D-Glucopyranose (5TMS)]	62	0.461	0.594	31.424	0.431	23	119	32	110	130	85 duplicate
16765	101 [832; Dopamine (4TMS)]	62	[812; D-Xylofuranose (4TMS)]	64	0.457	0.637	12.095	0.473	24	118	25	117	44	59 duplicate
11388	101 [832; Dopamine (4TMS)]	11	Succinic acid	64	0.456	0.642	8.335	0.474	25	117	24	118	7	57 duplicate
9150	101 [832; Dopamine (4TMS)]	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.455	0.627	6.882	0.361	26	116	29	113	4	129 original
16032	101 [832; Dopamine (4TMS)]	54	[NA]	55	0.433	0.661	13.034	0.422	27	115	22	120	50	91 duplicate
12752	101 [832; Dopamine (4TMS)]	22	[690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.409	0.628	13.205	0.450	28	114	28	114	52	77 duplicate
17361	101 [832; Dopamine (4TMS)]	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	0.398	0.475	16.228	0.424	29	113	41	101	71	90 duplicate
9128	101 [832; Dopamine (4TMS)]	106	[733; Threitol (4TMS)]	62	0.384	0.506	10.076	0.555	30	112	40	102	19	13 original
18016	101 [832; Dopamine (4TMS)]	80	[772; D-Glucose (5TMS)]	62	0.379	0.528	26.700	0.414	31	111	38	104	120	97 duplicate
9137	101 [832; Dopamine (4TMS)]	115	Glucose-6-phosphate	62	0.377	0.534	21.278	0.490	32	110	37	105	98	48 original
10043	101 [832; Dopamine (4TMS)]	1	[938; Sulfuric acid (2TMS)]	36	0.365	0.588	9.941	0.361	33	109	33	109	18	128 duplicate
13218	101 [832; Dopamine (4TMS)]	26	Citramalic acid	64	0.361	0.458	14.871	0.429	34	108	44	98	68	88 duplicate
9149	101 [832; Dopamine (4TMS)]	127	[777; Fructose-6-phosphate methoxyamine (8TMS)]	39	0.358	0.451	8.801	0.300	35	107	47	95	12	139 original
11772	101 [832; Dopamine (4TMS)]	14	Fumaric acid	64	0.353	0.613	11.849	0.474	36	106	30	112	39	58 duplicate
15402	101 [832; Dopamine (4TMS)]	47	[NA]	64	0.350	0.475	10.450	0.414	37	105	42	100	22	98 duplicate
17766	101 [832; Dopamine (4TMS)]	76	Fructose	64	0.343	0.561	21.614	0.506	38	104	35	107	102	32 duplicate
11517	101 [832; Dopamine (4TMS)]	12	Glyceric acid	63	0.335	0.611	13.468	0.427	39	103	31	111	56	89 duplicate
17893	101 [832; Dopamine (4TMS)]	78	Mannose	62	0.334	0.474	12.044	0.430	40	102	43	99	41	87 duplicate
17568	101 [832; Dopamine (4TMS)]	73	[708; Glucose methoxyamine (5TMS)]	57	0.330	0.343	11.755	0.493	41	101	57	85	38	43 duplicate
14208	101 [832; Dopamine (4TMS)]	35	Pyroglutamic acid	64	0.325	0.542	38.020	0.504	42	100	36	106	138	37 duplicate
13445	101 [832; Dopamine (4TMS)]	28	Malic acid	64	0.317	0.574	9.258	0.458	43	99	34	108	15	69 duplicate
14723	101 [832; Dopamine (4TMS)]	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.315	0.434	31.773	0.454	44	98	49	93	132	73 duplicate
12633	101 [832; Dopamine (4TMS)]	21	[678; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	64	0.297	0.420	14.693	0.410	46	96	50	92	67	100 duplicate

9139	101 [832; Dopamine (4TMS)] 117 [724; Glycerol (3TMS)]	58	0.291	0.356	11,306	0.408	47	95	58	86	29	102 original
9132	101 [832; Dopamine (4TMS)] 110 [715; Erythritol (4TMS)]	54	0.283	0.387	13,891	0.494	48	94	53	89	61	42 original
9143	101 [832; Dopamine (4TMS)] 121 [657; Erythritol (4TMS)]	55	0.278	0.308	16,974	0.387	49	93	60	82	78	116 original
19026	101 [832; Dopamine (4TMS)] 100 [857; Mannitol (6TMS)]	64	0.263	0.452	9,464	0.389	50	92	46	86	16	114 duplicate
18718	101 [832; Dopamine (4TMS)] 93 [607; Putrescine (4TMS)]	60	0.261	0.630	16,750	0.461	51	91	27	115	72	66 duplicate
10728	101 [832; Dopamine (4TMS)] 6 Glycerol	64	0.261	0.454	38,680	0.449	52	90	45	97	140	79 duplicate
9134	101 [832; Dopamine (4TMS)] 112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.261	0.383	19,281	0.442	53	89	54	88	88	81 original
9147	101 [832; Dopamine (4TMS)] 105 [892; Sucrose (6TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	0.241	0.517	28,119	0.489	54	88	39	103	125	47 original
9144	101 [832; Dopamine (4TMS)] 122 [644; Erythritol (4TMS)]	52	0.225	0.363	18,203	0.401	55	87	55	87	83	105 original
135												
9157	101 [832; Dopamine (4TMS)] [902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	0.190	0.266	12,053	0.385	56	85	63	79	42	117 original
14823	101 [832; Dopamine (4TMS)] 41 [638; Proline (2TMS)]	64	0.190	0.161	13,267	0.413	57	86	68	74	53	99 duplicate
9124	101 [832; Dopamine (4TMS)] 102 [904; Galactose methoxamine (5TMS)]	64	0.189	0.314	10,875	0.381	58	84	59	83	25	119 original
9142	101 [832; Dopamine (4TMS)] 120 [945; Uridine (3TMS)]	54	0.185	0.141	11,153	0.434	59	83	70	72	26	83 original
12392	101 [832; Dopamine (4TMS)] 19 Alanine (BP) (3TMS)	64	0.184	0.275	11,753	0.452	60	82	62	80	37	74 duplicate
9135	101 [832; Dopamine (4TMS)] 113 Galactose-6-phosphate	62	0.184	0.412	11,414	0.485	61	81	52	90	32	50 original
12270	101 [832; Dopamine (4TMS)] 18 [590; 1-Acetyl-2-thiohydantoin]	64	0.160	0.143	10,361	0.345	62	80	69	73	20	136 duplicate
18250	101 [832; Dopamine (4TMS)] 84 Mannitol	62	0.159	0.678	26,941	0.484	63	79	21	121	122	51 duplicate
15117	101 [832; Dopamine (4TMS)] 44 [910; 2-Ketogluconic acid methoxamine (4TMS)]	50	0.141	0.216	11,528	0.420	64	78	65	77	34	94 duplicate
9136	101 [832; Dopamine (4TMS)] 114 Fructose-6-phosphate	53	0.141	0.319	12,395	0.470	65	77	58	84	45	61 original
9145	101 [832; Dopamine (4TMS)] 123 [945; Galactofuranose-6-phosphate (7TMS)]	64	0.128	0.121	11,569	0.504	66	76	71	71	35	36 original
9126	101 [832; Dopamine (4TMS)] 104 [795; Erythritol (4TMS)]	63	0.121	0.113	11,385	0.507	67	75	72	70	31	31 original
17955	101 [832; Dopamine (4TMS)] 79 Glucose	64	0.110	0.301	31,956	0.505	68	74	61	81	134	33 duplicate
16920	101 [832; Dopamine (4TMS)] 64 [789; Tyramine (3TMS)]	63	0.108	0.101	10,707	0.399	69	73	74	68	24	106 duplicate
9140	101 [832; Dopamine (4TMS)] 118 [928; Glucopyranose-6-phosphate (8TMS)]	58	0.107	0.163	12,754	0.379	70	72	67	75	48	121 original
11898	101 [832; Dopamine (4TMS)] 15 Alanine	64	0.103	0.176	17,005	0.533	71	71	68	76	77	22 duplicate
9154	101 [832; Dopamine (4TMS)] 132 [895; Isomaltose methoxamine (8TMS)]	42	0.092	0.450	17,087	0.329	72	70	48	94	78	137 original
18306	101 [832; Dopamine (4TMS)] 85 [529; Methyldic acid (4TMS)]	48	0.087	0.255	5,625	0.492	73	69	64	78	3	44 duplicate
9138	101 [832; Dopamine (4TMS)] 116 [882; Pseudouridine (5TMS)]	30	0.085	0.091	9,019	0.410	74	68	75	67	13	101 original
18856	101 [832; Dopamine (4TMS)] 96 myo-Inositol	49	0.078	0.054	19,986	0.369	75	67	77	65	93	125 duplicate
17500	101 [832; Dopamine (4TMS)] 72 [919; D-Xylopyranose (4TMS)]	63	0.036	0.042	13,400	0.323	76	68	78	84	55	138 duplicate
9133	101 [832; Dopamine (4TMS)] 111 [583; Erythritol (4TMS)]	42	0.027	-0.003	22,395	0.281	77	65	80	62	108	140 original
9148	101 [832; Dopamine (4TMS)] 126 [559; Erythritol (4TMS)]	45	0.020	0.009	13,179	0.414	78	64	79	63	51	96 original
17635	101 [832; Dopamine (4TMS)] 74 [912; Tetradecanoic acid (1TMS)]	64	0.020	0.063	14,245	0.397	79	63	76	68	63	109 duplicate
15945	101 [832; Dopamine (4TMS)] 53 Glycerol-2-phosphate	64	0.003	0.104	14,595	0.358	80	62	73	69	68	131 duplicate
15020	101 [832; Dopamine (4TMS)] 43 [548; Leucine (2TBS)]	60	-0.021	-0.033	10,697	0.436	81	61	81	61	23	82 duplicate
18183	101 [832; Dopamine (4TMS)] 83 Sorbitol	58	-0.060	-0.392	21,887	0.497	82	60	96	46	103	40 duplicate
9158	101 [832; Dopamine (4TMS)] 136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.074	-0.211	7,478	0.253	83	59	87	55	5	141 original
9162	101 [832; Dopamine (4TMS)] 140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49	-0.085	-0.066	16,165	0.388	84	58	83	59	70	115 original
18571	101 [832; Dopamine (4TMS)] 90 [910; 8-(Z)-Hexadecenoic acid (1TMS)]	64	-0.098	-0.056	11,255	0.349	85	57	82	60	28	133 duplicate
9155	101 [832; Dopamine (4TMS)] 133 [855; Squalene]	64	-0.110	-0.372	13,706	0.389	86	56	95	47	59	113 original
9161	101 [832; Dopamine (4TMS)] 139 [700; Ergosta-5,7-dien-3-ol]	38	-0.118	-0.272	19,190	0.347	87	55	91	51	86	135 original
13332	101 [832; Dopamine (4TMS)] 27 [815; (E)-4-Methyl-5-hydroxy-3-pentan-2-one (1TMS)]	53	-0.151	-0.584	22,684	0.487	88	54	115	27	109	49 duplicate
10457	101 [832; Dopamine (4TMS)] 4 Phosphoric acid	51	-0.151	-0.467	33,392	0.447	89	53	101	41	136	80 duplicate
9160	101 [832; Dopamine (4TMS)] 138 [874; Ergosterol (1TMS)]	46	-0.165	-0.368	19,202	0.393	90	52	94	48	87	112 original
16843	101 [832; Dopamine (4TMS)] 63 Glutamine	52	-0.167	-0.469	21,929	0.540	91	51	102	40	104	18 duplicate
9131	101 [832; Dopamine (4TMS)] 109 Octadecanoic acid	64	-0.174	-0.155	22,803	0.355	92	50	84	58	110	132 original
[636; 4R-Acetaldo-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]												
16443	101 [832; Dopamine (4TMS)] 58 [709; 2,5-Diaminovalerolactam (2TMS)]	64	-0.183	-0.562	18,382	0.451	93	49	113	29	84	76 duplicate
13103	101 [832; Dopamine (4TMS)] 25 [708; 2,5-Diaminovalerolactam (2TMS)]	48	-0.188	-0.476	21,069	0.416	94	48	103	39	96	95 duplicate
15587	101 [832; Dopamine (4TMS)] 49 [877; Pyrophosphoric acid (4TMS)]	64	-0.202	-0.159	23,715	0.359	95	47	85	57	115	130 duplicate

9163	101 [832; Dopamine (4TMS)	141	Lanosta-8,24-dien-3-beta-ol	61	-0.215	-0.243	16,913	0.394	96	46	90	52	75	111 original
18765	101 [832; Dopamine (4TMS)	94	Hexadecanoic acid	64	-0.216	-0.230	21,513	0.365	97	45	88	54	101	127 duplicate
9141	101 [832; Dopamine (4TMS)	119	myo-Inositol-2-phosphate (7TMS)]	64	-0.221	-0.239	13,017	0.383	98	44	89	53	49	118 original
15213	101 [832; Dopamine (4TMS)	45	Homocysteine	61	-0.224	-0.201	24,326	0.374	99	43	86	56	117	123 duplicate
9129	101 [832; Dopamine (4TMS)	107	9-(Z)-Octadecanoic acid	64	-0.239	-0.354	15,103	0.348	100	42	93	49	69	134 original
17701	101 [832; Dopamine (4TMS)	75	Lysine	64	-0.255	-0.614	38,082	0.511	101	41	118	24	139	28 duplicate
18520	101 [832; Dopamine (4TMS)	89	775; Dopamine (4TMS)]	35	-0.261	-0.532	19,313	0.588	102	40	110	32	89	6 duplicate
15857	101 [832; Dopamine (4TMS)	52	[NA]	46	-0.268	-0.452	24,751	0.555	103	39	100	42	118	14 duplicate
9152	101 [832; Dopamine (4TMS)	130	Trehalose	63	-0.271	-0.485	28,029	0.372	104	38	105	37	124	124 original
16686	101 [832; Dopamine (4TMS)	61	[NA]	64	-0.289	-0.332	11,916	0.403	105	37	92	50	40	104 duplicate
10182	101 [832; Dopamine (4TMS)	2	Serine	62	-0.302	-0.692	23,612	0.487	106	36	127	15	113	48 duplicate
18811	101 [832; Dopamine (4TMS)	95	770; 3,4,6-Trisubstitutedphenylmethanolamine (5TMS)]	50	-0.308	-0.437	23,466	0.497	107	35	89	43	112	39 duplicate
18943	101 [832; Dopamine (4TMS)	98	697; Ribose-5-phosphate methoxyamine (5TMS)]	48	-0.314	-0.619	23,424	0.482	108	34	119	23	111	53 duplicate
12870	101 [832; Dopamine (4TMS)	23	Homoserine	64	-0.319	-0.597	17,239	0.450	109	33	116	26	79	78 duplicate
10995	101 [832; Dopamine (4TMS)	8	Isoleucine	55	-0.335	-0.665	22,531	0.469	110	32	125	17	107	63 duplicate
9159	101 [832; Dopamine (4TMS)	137	Ergosterol	64	-0.335	-0.521	18,083	0.379	111	31	109	33	81	120 original
17431	101 [832; Dopamine (4TMS)	71	731; Erythrose (3TMS)]	64	-0.337	-0.515	13,292	0.420	112	30	108	34	54	93 duplicate
14102	101 [832; Dopamine (4TMS)	34	Aspartic acid	64	-0.349	-0.476	31,778	0.408	113	29	104	38	133	103 duplicate
10593	101 [832; Dopamine (4TMS)	5	Leucine	45	-0.360	-0.422	11,508	0.512	114	28	97	45	33	27 duplicate
		124	734; 1-Monooleoylglycerol (2TMS); 1-											
9146	101 [832; Dopamine (4TMS)		Monoheptadecanoylglycerol (1TMS)]	59	-0.362	-0.511	26,562	0.369	115	27	107	35	119	126 original
17071	101 [832; Dopamine (4TMS)	66	Glyceric acid-3-phosphate	64	-0.362	-0.705	13,636	0.456	116	26	132	10	58	70 duplicate
14313	101 [832; Dopamine (4TMS)	36	596; N-Acetylglutamic acid (2TMS)]	64	-0.367	-0.728	28,485	0.470	117	25	134	8	126	62 duplicate
18135	101 [832; Dopamine (4TMS)	82	Lysine	39	-0.368	-0.550	18,533	0.625	118	24	111	31	90	3 duplicate
10862	101 [832; Dopamine (4TMS)	7	Threonine	64	-0.379	-0.660	28,728	0.452	119	23	124	18	127	75 duplicate
13778	101 [832; Dopamine (4TMS)	31	622; Parabanic acid (2TMS)]	64	-0.394	-0.650	16,907	0.422	120	22	123	19	74	92 duplicate
11127	101 [832; Dopamine (4TMS)	9	Proline	63	-0.399	-0.700	30,365	0.461	121	21	129	13	129	65 duplicate
13995	101 [832; Dopamine (4TMS)	33	Methionine	64	-0.400	-0.506	16,902	0.398	122	20	108	36	73	108 duplicate
15495	101 [832; Dopamine (4TMS)	48	Asparagine	64	-0.402	-0.560	18,193	0.504	123	19	112	30	82	35 duplicate
9130	101 [832; Dopamine (4TMS)	30	Octadecanoic acid	64	-0.423	-0.606	14,466	0.494	124	18	117	25	65	107 original
13987	101 [832; Dopamine (4TMS)	32	729; N,N-Dimethyllysine methyl ester]	63	-0.423	-0.729	23,641	0.494	125	17	135	7	114	41 duplicate
17218	101 [832; Dopamine (4TMS)	88	570; Hypoxanthine (2TMS)]	20	-0.432	-0.693	14,365	0.564	126	16	128	14	64	9 duplicate
9153	101 [832; Dopamine (4TMS)	131	626; 5-Methylthioadenosine (3TMS)]	55	-0.433	-0.436	19,793	0.509	127	15	98	44	92	29 original
17280	101 [832; Dopamine (4TMS)	69	Arginine	60	-0.441	-0.644	23,804	0.469	128	14	122	20	116	64 duplicate
16118	101 [832; Dopamine (4TMS)	55	612; 4-Aminobutyric acid (2TBS)]	43	-0.442	-0.628	21,393	0.588	129	13	120	22	99	7 duplicate
16525	101 [832; Dopamine (4TMS)	59	Omitrine; Arginine	64	-0.447	-0.643	39,376	0.454	130	12	121	21	141	72 duplicate
15768	101 [832; Dopamine (4TMS)	51	499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.457	-0.683	20,612	0.535	131	11	126	16	95	20 duplicate
13668	101 [832; Dopamine (4TMS)	30	815; Ethyl-3(2H)-thiophenone]	64	-0.465	-0.583	30,238	0.431	132	10	114	28	128	84 duplicate
12513	101 [832; Dopamine (4TMS)	20	619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.471	-0.701	13,748	0.651	133	9	130	12	60	1 duplicate
			826; beta-[[[5-methyl-2-thienyl)methyl]eneamino-											
17830	101 [832; Dopamine (4TMS)	77	benzeneacetic acid methyl ester]	62	-0.501	-0.719	31,440	0.484	134	8	133	9	131	52 duplicate
11258	101 [832; Dopamine (4TMS)	10	Glycine	64	-0.511	-0.703	21,068	0.531	135	7	131	11	97	25 duplicate
16606	101 [832; Dopamine (4TMS)	60	Glycerol-3-phosphate	64	-0.517	-0.754	21,468	0.480	136	6	139	3	100	56 duplicate
14417	101 [832; Dopamine (4TMS)	37	Phenylalanine	64	-0.520	-0.729	22,028	0.459	137	5	136	6	105	68 duplicate
17145	101 [832; Dopamine (4TMS)	67	Citric acid	64	-0.549	-0.733	22,623	0.430	138	4	137	5	108	86 duplicate
18076	101 [832; Dopamine (4TMS)	81	Tyrosine	64	-0.565	-0.828	34,645	0.611	139	3	141	1	137	5 duplicate
10320	101 [832; Dopamine (4TMS)	3	Ethanolamine	62	-0.578	-0.777	18,400	0.548	140	2	140	2	85	16 duplicate
14922	101 [832; Dopamine (4TMS)	42	Glutamic acid	60	-0.584	-0.737	32,175	0.470	141	1	138	4	135	60 duplicate
19027	102 [904; Galactose methox	100	857; Mannitol (6TMS)]	64	0.752	0.926	7,780	0.619	1	141	1	141	24	1 duplicate
9173	102 [904; Galactose methox	112	877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.732	0.854	11,928	0.576	2	140	2	140	53	5 original



9196	102 [904; Galactose methox	64	0.713	0.842	12,168	0.572	3	139	3	139	58	6 original
9193	102 [904; Galactose methox	42	0.654	0.753	12,788	0.563	4	138	7	135	65	9 original
13448	102 [904; Galactose methox	64	0.634	0.796	8,590	0.558	5	137	4	138	33	12 duplicate
9187	102 [904; Galactose methox	45	0.624	0.730	5,960	0.580	6	136	13	129	10	3 original
9176	102 [904; Galactose methox	62	0.617	0.665	25,085	0.571	7	135	28	114	118	7 original
9177	102 [904; Galactose methox	30	0.605	0.570	6,968	0.542	8	134	51	81	16	81 original
14209	102 [904; Galactose methox	64	0.604	0.641	42,281	0.537	9	133	31	111	140	29 duplicate
14724	102 [904; Galactose methox	64	0.566	0.736	35,444	0.515	10	132	11	131	134	44 duplicate
11518	102 [904; Galactose methox	63	0.551	0.746	6,148	0.550	11	131	9	133	12	17 duplicate
11773	102 [904; Galactose methox	64	0.551	0.728	4,165	0.528	12	130	14	128	5	37 duplicate
17767	102 [904; Galactose methox	64	0.547	0.605	26,089	0.528	13	129	44	98	120	36 duplicate
15118	102 [904; Galactose methox	50	0.536	0.748	9,006	0.540	14	128	8	134	38	27 duplicate
16766	102 [904; Galactose methox	64	0.536	0.670	14,189	0.538	15	127	27	115	72	28 duplicate
17636	102 [904; Galactose methox	64	0.533	0.674	7,982	0.460	16	126	25	117	26	70 duplicate
9183	102 [904; Galactose methox	52	0.528	0.708	12,285	0.558	17	125	19	123	60	13 original
9182	102 [904; Galactose methox	55	0.522	0.632	10,268	0.548	18	124	37	105	45	18 original
9178	102 [904; Galactose methox	56	0.512	0.689	6,996	0.580	19	123	22	120	18	4 original
9167	102 [904; Galactose methox	62	0.511	0.637	10,217	0.542	20	122	34	108	44	23 original
11389	102 [904; Galactose methox	64	0.509	0.726	6,759	0.501	21	121	15	127	15	51 duplicate
9172	102 [904; Galactose methox	42	0.508	0.770	16,381	0.503	22	120	5	137	87	50 original
13558	102 [904; Galactose methox	64	0.506	0.745	3,031	0.537	23	119	10	132	2	30 duplicate
9171	102 [904; Galactose methox	54	0.498	0.609	10,145	0.554	25	117	42	100	43	16 original
14521	102 [904; Galactose methox	38	0.498	0.756	6,811	0.558	26	116	6	136	14	11 duplicate
12753	102 [904; Galactose methox	52	0.490	0.712	8,538	0.555	27	115	17	125	32	14 duplicate
18307	102 [904; Galactose methox	48	0.489	0.699	3,316	0.494	28	114	20	122	3	55 duplicate
12634	102 [904; Galactose methox	62	0.486	0.636	16,824	0.516	29	113	35	107	90	43 duplicate
17894	102 [904; Galactose methox	64	0.485	0.610	8,726	0.481	30	112	40	102	35	68 duplicate
9175	102 [904; Galactose methox	53	0.485	0.673	5,722	0.522	31	111	28	116	9	38 original
16033	102 [904; Galactose methox	55	0.471	0.733	8,661	0.507	32	110	12	130	34	48 duplicate
9181	102 [904; Galactose methox	54	0.463	0.232	11,635	0.571	33	109	76	66	50	8 original
13219	102 [904; Galactose methox	64	0.459	0.595	16,727	0.494	34	108	45	97	89	54 duplicate
12988	102 [904; Galactose methox	64	0.457	0.680	32,823	0.542	35	107	23	119	131	24 duplicate
18362	102 [904; Galactose methox	61	0.456	0.618	22,120	0.559	36	106	39	103	112	10 duplicate
9174	102 [904; Galactose methox	62	0.455	0.591	6,109	0.455	37	105	48	84	11	74 original
9186	102 [904; Galactose methox	64	0.454	0.474	32,729	0.464	38	104	57	85	130	66 original
12024	102 [904; Galactose methox	64	0.439	0.697	18,040	0.546	39	103	21	121	99	19 duplicate
17569	102 [904; Galactose methox	57	0.430	0.624	8,214	0.405	40	102	38	104	29	107 duplicate
16277	102 [904; Galactose methox	64	0.429	0.646	9,467	0.535	41	101	30	112	41	33 duplicate
14623	102 [904; Galactose methox	63	0.428	0.709	16,139	0.534	42	100	18	124	85	34 duplicate
15309	102 [904; Galactose methox	64	0.427	0.635	17,609	0.529	43	99	38	106	95	35 duplicate
18469	102 [904; Galactose methox	84	0.423	0.610	11,849	0.537	44	98	41	101	52	31 duplicate
12271	102 [904; Galactose methox	84	0.417	0.548	6,966	0.432	45	97	52	90	17	87 duplicate
18857	102 [904; Galactose methox	49	0.415	0.279	15,422	0.339	46	96	73	69	79	135 duplicate
9195	102 [904; Galactose methox	64	0.414	0.648	25,575	0.536	47	95	29	113	119	32 original
16997	102 [904; Galactose methox	63	0.398	0.678	12,312	0.544	48	94	24	118	61	21 duplicate
17362	102 [904; Galactose methox	57	0.397	0.444	18,884	0.363	49	93	59	83	102	127 duplicate
13361	102 [904; Galactose methox	55	0.393	0.608	13,788	0.510	50	92	43	89	70	46 duplicate
9189	102 [904; Galactose methox	45	0.390	0.714	7,599	0.522	51	91	16	126	23	39 original
12148	102 [904; Galactose methox	64	0.377	0.639	17,869	0.498	52	90	32	110	97	53 duplicate

18671	102 [904; Galactose methox	92 [680; Glycerol-2-phosphate (4TMS)]	54 0.367	0.382	8,211	0.467	53	89	61	81	28	65 duplicate
15679	102 [904; Galactose methox	50 [746; Ribonic acid-1,4-lactone (3TMS)]	61 0.366	0.581	14,411	0.522	54	88	50	92	74	40 duplicate
9170	102 [904; Galactose methox	109 Octadecanoic acid	64 0.365	0.531	22,663	0.401	55	87	53	89	114	110 original
18194	102 [904; Galactose methox	83 Sorbitol	58 0.364	-0.039	21,959	0.326	56	86	90	52	110	139 duplicate
11648	102 [904; Galactose methox	13 Uracil	64 0.358	0.638	16,417	0.544	57	85	33	109	88	20 duplicate
129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-O-												
9190	102 [904; Galactose methox	Glc]	59 0.347	0.592	11,074	0.555	58	84	46	96	49	15 original
18766	102 [904; Galactose methox	94 Hexadecanoic acid	64 0.344	0.497	22,082	0.407	59	83	55	87	111	105 duplicate
9188	102 [904; Galactose methox	127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	39 0.336	0.505	4,476	0.583	60	82	54	88	6	2 original
9164	102 [904; Galactose methox	103 [648; Ethylamine (2TMS)]	63 0.308	0.470	14,275	0.449	61	81	58	84	73	78 original
9184	102 [904; Galactose methox	123 [945; Galactofuranose-6-phosphate (7TMS)]	64 0.288	0.344	10,818	0.412	62	80	63	79	47	99 original
12393	102 [904; Galactose methox	19 Alanine (BP) (3TMS)	64 0.270	0.354	12,120	0.424	63	78	62	80	57	91 duplicate
9201	102 [904; Galactose methox	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49 0.269	0.292	11,765	0.460	64	78	70	72	51	69 original
17432	102 [904; Galactose methox	71 [731; Erythrose (3TMS)]	64 0.265	0.268	12,266	0.478	65	77	74	68	59	61 duplicate
9199	102 [904; Galactose methox	138 [674; Ergosterol (1TMS)]	46 0.264	0.305	12,589	0.469	66	76	68	74	84	63 original
9202	102 [904; Galactose methox	141 Lanosta-8,24-dien-3-beta-ol	61 0.251	0.329	9,788	0.422	67	75	65	77	42	92 original
9194	102 [904; Galactose methox	141 Lanosta-8,24-dien-3-beta-ol	61 0.251	0.329	9,788	0.422	67	75	65	77	42	92 original
18986	102 [904; Galactose methox	99 [682; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41 0.232	0.586	8,404	0.541	69	73	49	93	31	26 duplicate
9165	102 [904; Galactose methox	104 [795; Erythritol (4TMS)]	63 0.231	0.327	7,008	0.366	70	72	68	76	19	123 original
10729	102 [904; Galactose methox	6 Glycerol	64 0.226	0.343	42,882	0.378	71	71	64	78	141	119 duplicate
9166	102 [904; Galactose methox	105 [705; 2-Ketogluconic acid (5TMS)]	48 0.218	0.476	11,968	0.487	72	70	56	86	55	57 original
16921	102 [904; Galactose methox	64 [789; Tyramine (3TMS)]	63 0.204	0.389	3,420	0.409	73	69	60	82	4	102 duplicate
9198	102 [904; Galactose methox	137 Ergosterol	64 0.193	0.153	14,784	0.365	74	68	82	60	75	124 original
19067	102 [904; Galactose methox	101 [832; Dopamine (4TMS)]	64 0.189	0.314	10,875	0.381	75	68	67	75	48	117 duplicate
14824	102 [904; Galactose methox	41 [639; Proline (2TMS)]	64 0.189	0.201	14,114	0.429	76	67	78	64	71	90 duplicate
18622	102 [904; Galactose methox	91 [766; beta-D-Methylglucopyranoside (4TMS)]	64 0.182	0.303	17,378	0.380	77	65	69	73	93	118 duplicate
18251	102 [904; Galactose methox	84 Mannitol	62 0.172	0.280	32,594	0.395	78	64	72	70	129	114 duplicate
18901	102 [904; Galactose methox	97 [756; beta-D-Methylglucopyranoside (4TMS)]	52 0.151	0.260	21,555	0.411	79	63	75	67	109	100 duplicate
11899	102 [904; Galactose methox	15 Alanine	64 0.150	0.141	19,198	0.477	80	62	84	58	103	62 duplicate
9180	102 [904; Galactose methox	119 [931; myo-Inositol-2-phosphate (7TMS)]	64 0.133	0.143	8,094	0.378	81	61	83	59	27	120 original
9197	102 [904; Galactose methox	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17 0.103	0.192	2,986	0.486	82	60	79	63	1	58 original
18416	102 [904; Galactose methox	87 [945; beta-D-Glucopyranose (5TMS)]	62 0.099	0.190	36,351	0.442	83	59	81	61	137	80 duplicate
18719	102 [904; Galactose methox	93 [607; Putrescine (4TMS)]	60 0.095	0.192	13,048	0.387	84	58	80	82	69	122 duplicate
17858	102 [904; Galactose methox	79 Glucose	64 0.093	0.285	35,950	0.430	85	57	71	138	89 duplicate	
9168	102 [904; Galactose methox	107 9-(Z)-Octadecenoic acid	64 0.063	-0.015	15,136	0.332	86	56	89	53	77	138 original
18572	102 [904; Galactose methox	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	64 0.060	0.086	7,213	0.347	87	55	85	57	20	132 duplicate
9200	102 [904; Galactose methox	139 [700; Ergosta-5,7-dien-3-ol]	38 0.055	-0.115	14,899	0.438	88	54	93	49	76	83 original
124 [734; 1-Monooleoylglycerol (2TMS); 1-												
9185	102 [904; Galactose methox	Monohexadecenoylglycerol (1TMS)]	59 0.030	-0.137	19,406	0.352	89	53	95	47	104	130 original
10863	102 [904; Galactose methox	7 Threonine	64 -0.015	-0.132	31,241	0.349	90	52	94	48	124	131 duplicate
17146	102 [904; Galactose methox	67 Citric acid	64 -0.032	-0.048	24,676	0.344	91	51	91	51	117	134 duplicate
16607	102 [904; Galactose methox	60 Glycerol-3-phosphate	64 -0.036	-0.067	22,332	0.409	92	50	92	50	113	103 duplicate
18017	102 [904; Galactose methox	80 [772; D-Glucose (5TMS)]	62 -0.046	0.047	31,837	0.382	93	49	87	55	128	116 duplicate
14418	102 [904; Galactose methox	37 Phenylalanine	64 -0.059	-0.147	23,673	0.414	94	48	96	46	116	97 duplicate
10044	102 [904; Galactose methox	1 [938; Sulfuric acid (2TMS)]	38 -0.063	0.006	7,831	0.542	95	47	88	54	25	25 duplicate
16687	102 [904; Galactose methox	61 [NA]	64 -0.129	0.074	5,544	0.409	96	46	88	56	8	104 duplicate
9169	102 [904; Galactose methox	108 Octadecenoic acid	64 -0.146	-0.256	6,269	0.384	97	45	88	44	13	115 original
15403	102 [904; Galactose methox	47 [NA]	64 -0.151	-0.336	11,962	0.456	98	44	109	33	54	72 duplicate
9179	102 [904; Galactose methox	118 [928; Glucopyranose-6-phosphate (6TMS)]	58 -0.157	-0.309	8,753	0.452	99	43	106	36	36	77 original
15858	102 [904; Galactose methox	52 [NA]	46 -0.161	-0.330	17,107	0.449	100	42	108	34	91	79 duplicate
10996	102 [904; Galactose methox	8 Isoleucine	55 -0.162	-0.236	20,031	0.320	101	41	97	45	105	140 duplicate

18812	102 [904; Galactose methox	95	[770; 3,4,6-Trisubstitutedphenylmethanamine (5TMS)]	50	-0.162	-0.273	15.592	0.359	102	40	101	41	80	129 duplicate
15946	102 [904; Galactose methox	53	Glycerol-2-phosphate	64	-0.165	-0.293	7.357	0.337	103	39	103	39	21	136 duplicate
10321	102 [904; Galactose methox	3	Ethanolamine	62	-0.186	-0.342	9.246	0.411	104	38	110	32	39	101 duplicate
16119	102 [904; Galactose methox	55	[612; 4-Aminobutyric acid (2TBS)]	43	-0.187	-0.296	18.438	0.335	105	37	104	38	100	137 duplicate
14314	102 [904; Galactose methox	36	[596; N-Acetylglutamic acid (2TMS)]	64	-0.189	-0.292	29.904	0.364	108	36	102	40	122	126 duplicate
17072	102 [904; Galactose methox	66	Glyceric acid-3-phosphate	64	-0.208	-0.268	5.182	0.416	107	35	100	42	7	95 duplicate
15769	102 [904; Galactose methox	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.235	-0.409	16.368	0.480	108	34	121	21	86	60 duplicate
18077	102 [904; Galactose methox	81	Tyrosine	64	-0.237	-0.406	35.528	0.434	109	33	120	22	135	85 duplicate
11128	102 [904; Galactose methox	9	Proline	63	-0.248	-0.354	29.220	0.376	110	32	114	28	121	121 duplicate
16444	102 [904; Galactose methox	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	-0.253	-0.260	17.216	0.364	111	31	99	43	92	125 duplicate
9191	102 [904; Galactose methox	130	Trehalose	63	-0.254	-0.347	30.949	0.399	112	30	112	30	123	112 original
10458	102 [904; Galactose methox	4	Phosphoric acid	51	-0.256	-0.301	34.535	0.310	113	29	105	37	133	141 duplicate
17831	102 [904; Galactose methox	77	[826; beta-[[[5-methyl-2-thienyl)methyl]eneamino-benzeneacetic acid methyl ester]	62	-0.258	-0.367	31.346	0.399	114	28	116	26	125	111 duplicate
17702	102 [904; Galactose methox	75	Lysine	64	-0.258	-0.314	40.977	0.345	115	26	107	35	138	133 duplicate
13669	102 [904; Galactose methox	30	[815; Ethyl-3(2H)-thiophenone]	64	-0.258	-0.398	31.363	0.360	116	27	118	24	126	128 duplicate
14103	102 [904; Galactose methox	34	Aspartic acid	64	-0.267	-0.347	34.123	0.413	117	25	111	31	132	98 duplicate
12514	102 [904; Galactose methox	20	[619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.273	-0.436	12.877	0.456	118	24	122	20	66	73 duplicate
13779	102 [904; Galactose methox	31	[622; Parabanic acid (2TMS)]	64	-0.278	-0.401	8.277	0.453	119	23	119	23	30	75 duplicate
13998	102 [904; Galactose methox	33	Methionine	64	-0.280	-0.441	12.057	0.435	120	22	123	19	56	84 duplicate
15214	102 [904; Galactose methox	45	Homocysteine	61	-0.284	-0.361	17.623	0.398	121	21	115	27	96	113 duplicate
17501	102 [904; Galactose methox	72	[919; D-Xylopyranose (4TMS)]	63	-0.288	-0.531	9.283	0.406	122	20	132	10	40	106 duplicate
10594	102 [904; Galactose methox	5	Leucine	45	-0.291	-0.538	10.276	0.463	123	19	134	8	46	67 duplicate
10183	102 [904; Galactose methox	2	Serine	62	-0.298	-0.352	20.481	0.419	124	18	113	29	107	94 duplicate
12871	102 [904; Galactose methox	23	Homoserine	64	-0.311	-0.615	12.383	0.503	125	17	138	4	62	49 duplicate
17219	102 [904; Galactose methox	68	[570; Hypoxanthine (2TMS)]	20	-0.316	-0.524	12.446	0.452	126	16	131	11	63	76 duplicate
11259	102 [904; Galactose methox	69	Glycine	64	-0.319	-0.556	20.503	0.543	127	15	135	7	108	22 duplicate
15496	102 [904; Galactose methox	48	Asparagine	60	-0.328	-0.595	23.100	0.516	128	14	136	6	115	42 duplicate
16526	102 [904; Galactose methox	59	Omithine; Arginine	64	-0.329	-0.476	12.973	0.494	129	13	126	16	67	56 duplicate
13888	102 [904; Galactose methox	42	Glutamic acid	64	-0.339	-0.392	42.277	0.415	130	12	117	25	139	86 duplicate
14923	102 [904; Galactose methox	32	[729; N,N-Dimethyllysine methyl ester]	63	-0.341	-0.517	15.655	0.517	131	11	129	13	82	41 duplicate
18521	102 [904; Galactose methox	89	[775; Dopamine (4TMS)]	60	-0.344	-0.479	31.504	0.439	132	10	128	14	127	82 duplicate
18944	102 [904; Galactose methox	98	[697; Ribose-5-phosphate methoxamine (5TMS)]	35	-0.351	-0.536	15.947	0.459	133	9	133	9	83	71 duplicate
16844	102 [904; Galactose methox	63	Glutamine	48	-0.353	-0.616	16.020	0.500	134	8	139	3	84	52 duplicate
15588	102 [904; Galactose methox	49	[877; Pyrophosphoric acid (4TMS)]	52	-0.354	-0.444	15.642	0.513	135	7	124	18	81	45 duplicate
13333	102 [904; Galactose methox	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	64	-0.374	-0.463	17.908	0.403	136	6	125	17	98	108 duplicate
9192	102 [904; Galactose methox	131	[826; 5-Methylthioadenosine (3TMS)]	53	-0.393	-0.612	17.505	0.484	137	5	137	5	94	59 duplicate
18136	102 [904; Galactose methox	82	Lysine	55	-0.407	-0.519	13.004	0.431	138	4	130	12	68	88 original
15021	102 [904; Galactose methox	43	[548; Leucine (2TBS)]	39	-0.414	-0.479	8.810	0.468	139	3	140	2	101	64 duplicate
13104	102 [904; Galactose methox	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.441	-0.645	18.494	0.468	139	3	140	2	101	64 duplicate
18902	102 [904; Galactose methox	97	[756; beta-D-Methylglucopyranoside (4TMS)]	48	-0.543	-0.717	15.222	0.509	141	1	141	1	78	109 duplicate
9204	103 [648; Ethylamine (2TMS	105	[705; 2-Ketogluconic acid (5TMS)]	52	0.846	0.913	9.524	0.592	1	141	3	139	12	13 duplicate
19068	103 [648; Ethylamine (2TMS	101	[832; Dopamine (4TMS)]	48	0.817	0.854	4.669	0.676	2	140	2	140	1	1 original
18672	103 [648; Ethylamine (2TMS	92	[680; Glycerol-2-phosphate (4TMS)]	63	0.808	0.958	5.254	0.650	3	139	1	141	2	3 duplicate
18623	103 [648; Ethylamine (2TMS	81	[766; beta-D-Methylglucopyranoside (4TMS)]	53	0.769	0.875	11.056	0.466	4	138	30	112	19	86 duplicate
9233	103 [648; Ethylamine (2TMS	134	Isomaltose	63	0.733	0.909	7.243	0.640	5	137	4	138	3	4 duplicate
16278	103 [648; Ethylamine (2TMS	56	[829; Optic acid (3TMS)]	63	0.711	0.857	18.967	0.590	6	136	6	136	68	15 original
16998	103 [648; Ethylamine (2TMS	65	[646; 3-Deoxyglucitol (5TMS)]	62	0.693	0.846	10.480	0.597	7	135	9	133	15	11 duplicate
					0.676	0.829	10.761	0.565	8	134	11	131	18	23 duplicate

15310	103 [648; Ethylamine (2TMS 46	Arabinose	63	0.668	0.835	9.439	0.568	9	133	10	132	11	21 duplicate
11647	103 [648; Ethylamine (2TMS 13	Uracil	63	0.665	0.864	10.632	0.604	10	132	5	137	17	9 duplicate
18470	103 [648; Ethylamine (2TMS 88	Gluconic acid	63	0.659	0.800	8.421	0.573	11	131	18	124	6	17 duplicate
12025	103 [648; Ethylamine (2TMS 18	[644; 2-Methyl-1,3-butanediol (2TMS)]	63	0.653	0.853	13.543	0.605	12	130	7	135	34	8 duplicate
	129 [640; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]												
9228	103 [648; Ethylamine (2TMS	Glc]	59	0.649	0.822	9.202	0.548	13	129	13	129	8	30 original
12989	103 [648; Ethylamine (2TMS 24	[725; 2-Ketooctanoic acid (2TMS)]	63	0.645	0.849	26.316	0.608	14	128	8	134	116	7 duplicate
	103 [648; Ethylamine (2TMS												
16362	57 [757; 2-Desoxy-pentose-3-yl-ose dimethoxyamine (2TMS)]		55	0.626	0.774	8.992	0.503	15	127	21	121	7	64 duplicate
12149	103 [648; Ethylamine (2TMS 17	[700; 2-methyl-1,2-propanediol (2TMS)]	63	0.616	0.821	12.993	0.537	16	126	15	127	29	38 duplicate
18363	103 [648; Ethylamine (2TMS 85	[793; D-Galactono-1,4-lactone (4TMS)]	60	0.614	0.795	14.235	0.579	17	125	20	122	42	16 duplicate
14624	103 [648; Ethylamine (2TMS 39	[829; 1-Phenylethanol (1TMS)]	62	0.601	0.821	9.202	0.541	18	124	14	128	9	37 duplicate
18987	103 [648; Ethylamine (2TMS 99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	0.600	0.798	15.380	0.519	19	123	19	123	54	47 duplicate
13559	103 [648; Ethylamine (2TMS 29	Erythritol	63	0.585	0.824	12.324	0.546	20	122	12	130	25	33 duplicate
14522	103 [648; Ethylamine (2TMS 38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	63	0.576	0.812	10.231	0.568	21	121	17	125	14	20 duplicate
15680	103 [648; Ethylamine (2TMS 50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	0.565	0.816	22.899	0.562	22	120	16	126	102	28 duplicate
16034	103 [648; Ethylamine (2TMS 54	[NA]	54	0.560	0.762	15.078	0.474	23	119	23	119	48	81 duplicate
9227	103 [648; Ethylamine (2TMS 128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	44	0.556	0.771	8.023	0.515	24	118	22	120	5	51 original
16767	103 [648; Ethylamine (2TMS 82	[812; D-Xylofuranose (4TMS)]	63	0.548	0.741	11.164	0.516	26	116	27	115	20	50 duplicate
11390	103 [648; Ethylamine (2TMS 11	Succinic acid	63	0.543	0.741	11.164	0.516	26	116	27	115	20	50 duplicate
12754	103 [648; Ethylamine (2TMS 22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.484	0.754	15.552	0.543	27	115	24	118	56	36 duplicate
9214	103 [648; Ethylamine (2TMS 115	Glucose-6-phosphate	61	0.478	0.646	20.114	0.552	28	114	33	109	82	29 original
11774	103 [648; Ethylamine (2TMS 14	Fumaric acid	61	0.476	0.747	15.171	0.539	29	113	25	117	50	38 duplicate
9205	103 [648; Ethylamine (2TMS 106	[733; Threitol (4TMS)]	61	0.472	0.638	10.575	0.611	30	112	35	107	16	6 original
17363	103 [648; Ethylamine (2TMS 70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	56	0.465	0.518	16.227	0.463	31	111	52	90	63	90 duplicate
11519	103 [648; Ethylamine (2TMS 12	Glycetic acid	62	0.464	0.732	16.641	0.512	32	110	28	114	67	54 duplicate
17768	103 [648; Ethylamine (2TMS 76	Fructose	63	0.445	0.667	19.976	0.527	33	109	31	111	80	41 duplicate
17895	103 [648; Ethylamine (2TMS 78	Mannose	61	0.439	0.598	13.577	0.489	34	108	39	103	35	71 duplicate
18417	103 [648; Ethylamine (2TMS 87	[945; beta-D-Glucopyranose (5TMS)]	61	0.438	0.611	29.984	0.461	35	107	37	105	128	84 duplicate
13447	103 [648; Ethylamine (2TMS 127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	63	0.438	0.720	11.473	0.546	36	106	29	113	21	32 duplicate
9226	103 [648; Ethylamine (2TMS 73	[708; Glucose methoxyamine (6TMS)]	39	0.436	0.594	11.739	0.420	37	105	40	102	22	113 original
17570	103 [648; Ethylamine (2TMS 35	Pyroglutamic acid	56	0.416	0.477	12.701	0.463	39	103	57	85	28	92 duplicate
14210	103 [648; Ethylamine (2TMS 26	Citramalic acid	63	0.412	0.639	36.558	0.509	40	102	34	108	138	58 duplicate
13220	103 [648; Ethylamine (2TMS 117	[724; Glyceral (3TMS)]	63	0.401	0.568	15.741	0.500	41	101	45	97	60	67 duplicate
9216	103 [648; Ethylamine (2TMS 40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	56	0.395	0.521	13.151	0.486	42	100	51	91	30	73 original
14725	103 [648; Ethylamine (2TMS 110	[715; Erythritol (4TMS)]	63	0.391	0.585	30.750	0.505	43	99	43	99	129	62 duplicate
9209	103 [648; Ethylamine (2TMS 100	[857; Mannitol (6TMS)]	54	0.378	0.540	15.312	0.563	44	98	48	94	53	25 original
19028	103 [648; Ethylamine (2TMS 21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	63	0.368	0.587	11.855	0.464	45	97	41	101	23	88 duplicate
12635	103 [648; Ethylamine (2TMS 121	[657; Erythritol (4TMS)]	63	0.365	0.536	15.123	0.476	46	96	49	93	49	79 duplicate
10045	103 [648; Ethylamine (2TMS 1	[938; Sulfuric acid (2TMS)]	55	0.351	0.451	19.759	0.441	47	95	60	82	77	102 original
9211	103 [648; Ethylamine (2TMS 112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	36	0.343	0.585	13.393	0.475	48	94	42	100	33	80 duplicate
18018	103 [648; Ethylamine (2TMS 80	[772; D-Glucose (5TMS)]	62	0.339	0.524	22.583	0.521	49	93	50	92	98	44 original
9221	103 [648; Ethylamine (2TMS 122	[644; Erythritol (4TMS)]	52	0.321	0.509	25.851	0.432	50	92	53	89	112	107 duplicate
19107	103 [648; Ethylamine (2TMS 102	[904; Galactose methoxyamine (5TMS)]	53	0.306	0.470	14.275	0.449	52	90	58	84	44	81 original
18720	103 [648; Ethylamine (2TMS 93	[607; Putrescine (4TMS)]	59	0.303	0.603	19.847	0.437	53	89	38	104	78	98 duplicate
9224	103 [648; Ethylamine (2TMS 125	[892; Sucrose (6TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	63	0.302	0.574	28.725	0.502	54	88	44	98	118	66 original
9219	103 [648; Ethylamine (2TMS 120	[945; Uridine (3TMS)]	54	0.290	0.183	12.803	0.509	55	87	73	69	27	56 original
10730	103 [648; Ethylamine (2TMS 6	Glycerol	63	0.286	0.502	37.334	0.468	56	86	56	88	140	85 duplicate
9212	103 [648; Ethylamine (2TMS 113	Galactose-6-phosphate	61	0.278	0.505	14.037	0.512	57	85	55	87	40	53 original
15404	103 [648; Ethylamine (2TMS 47	[NA]	63	0.270	0.378	13.976	0.437	58	84	63	79	39	104 duplicate

9234	103 [648; Ethylamine (2TMS	135	63	0.264	0.412	13.901	0.456	59	83	62	80	37	96 original
15119	103 [648; Ethylamine (2TMS	44	50	0.256	0.418	12.252	0.476	60	82	61	81	24	78 duplicate
18308	103 [648; Ethylamine (2TMS	85	47	0.254	0.507	7.541	0.462	61	81	54	88	4	93 duplicate
9213	103 [648; Ethylamine (2TMS	114	53	0.235	0.458	15.268	0.507	62	80	59	83	52	59 original
12394	103 [648; Ethylamine (2TMS	19	63	0.215	0.366	13.175	0.492	63	79	64	78	31	70 duplicate
12272	103 [648; Ethylamine (2TMS	18	63	0.208	0.245	13.214	0.416	64	78	68	74	32	115 duplicate
9203	103 [648; Ethylamine (2TMS	104	62	0.204	0.222	13.944	0.509	65	77	70	72	38	57 original
9215	103 [648; Ethylamine (2TMS	116	30	0.191	0.269	9.729	0.375	66	76	68	76	13	130 original
9231	103 [648; Ethylamine (2TMS	132	42	0.189	0.620	18.909	0.429	67	75	36	106	74	109 original
14825	103 [648; Ethylamine (2TMS	41	63	0.188	0.236	14.584	0.444	68	74	69	73	47	100 duplicate
9222	103 [648; Ethylamine (2TMS	123	63	0.183	0.218	13.608	0.543	69	73	71	71	36	35 original
18252	103 [648; Ethylamine (2TMS	84	61	0.150	0.650	25.842	0.519	70	72	32	110	111	45 duplicate
9225	103 [648; Ethylamine (2TMS	126	45	0.147	0.209	15.612	0.488	71	71	72	70	57	72 original
17637	103 [648; Ethylamine (2TMS	74	63	0.127	0.259	15.805	0.455	72	70	67	75	61	87 duplicate
18858	103 [648; Ethylamine (2TMS	96	48	0.119	0.061	22.697	0.361	73	69	80	62	100	134 duplicate
9210	103 [648; Ethylamine (2TMS	111	42	0.103	0.157	25.454	0.328	74	68	75	67	108	139 original
18922	103 [648; Ethylamine (2TMS	64	62	0.096	0.136	14.470	0.375	75	67	76	68	45	129 duplicate
11900	103 [648; Ethylamine (2TMS	15	63	0.087	0.174	17.747	0.554	76	68	74	68	71	28 duplicate
17957	103 [648; Ethylamine (2TMS	79	63	0.079	0.344	30.865	0.546	77	65	65	77	131	34 duplicate
18195	103 [648; Ethylamine (2TMS	83	57	0.051	-0.385	22.665	0.465	78	64	97	45	99	87 duplicate
9217	103 [648; Ethylamine (2TMS	118	58	0.034	0.102	16.515	0.357	79	63	77	65	66	135 original
9239	103 [648; Ethylamine (2TMS	140	48	0.028	0.100	19.260	0.387	80	62	78	64	75	125 original
9235	103 [648; Ethylamine (2TMS	136	17	0.015	-0.101	9.368	0.261	81	61	87	55	10	141 original
9232	103 [648; Ethylamine (2TMS	133	63	-0.017	-0.213	16.340	0.385	82	60	91	51	64	127 original
15947	103 [648; Ethylamine (2TMS	53	37	-0.020	-0.078	18.480	0.374	83	59	79	63	73	131 duplicate
9236	103 [648; Ethylamine (2TMS	139	63	-0.039	-0.144	22.524	0.321	84	58	89	53	98	140 original
18573	103 [648; Ethylamine (2TMS	90	63	-0.040	0.033	14.256	0.341	85	57	82	60	43	138 duplicate
17502	103 [648; Ethylamine (2TMS	72	62	-0.050	-0.060	17.453	0.352	86	56	84	58	69	137 duplicate
9208	103 [648; Ethylamine (2TMS	109	63	-0.054	0.040	22.112	0.390	87	55	81	61	90	124 original
15022	103 [648; Ethylamine (2TMS	43	59	-0.059	-0.099	14.170	0.429	88	54	86	58	41	110 duplicate
9240	103 [648; Ethylamine (2TMS	141	60	-0.089	-0.068	19.942	0.376	89	53	85	57	79	128 original
9237	103 [648; Ethylamine (2TMS	138	45	-0.113	-0.205	22.362	0.399	90	52	90	52	94	119 original
18767	103 [648; Ethylamine (2TMS	94	63	-0.115	-0.032	21.124	0.385	91	51	83	59	86	126 duplicate
16845	103 [648; Ethylamine (2TMS	63	63	-0.149	-0.119	15.653	0.392	92	50	88	54	59	122 original
9206	103 [648; Ethylamine (2TMS	63	51	-0.151	-0.551	25.807	0.558	93	49	106	36	110	27 duplicate
10459	103 [648; Ethylamine (2TMS	107	63	-0.178	-0.249	16.399	0.371	94	48	92	50	65	132 original
9236	103 [648; Ethylamine (2TMS	4	50	-0.213	-0.476	33.003	0.403	95	47	102	40	135	117 duplicate
15859	103 [648; Ethylamine (2TMS	52	63	-0.221	-0.357	19.327	0.362	96	48	98	48	76	133 original
13334	103 [648; Ethylamine (2TMS	52	45	-0.232	-0.498	26.268	0.597	97	45	103	39	123	12 duplicate
16445	103 [648; Ethylamine (2TMS	58	52	-0.249	-0.680	25.915	0.519	98	44	121	21	114	48 duplicate
18813	103 [648; Ethylamine (2TMS	95	63	-0.259	-0.555	20.200	0.449	99	43	107	35	83	99 duplicate
17433	103 [648; Ethylamine (2TMS	71	49	-0.264	-0.455	26.097	0.529	100	42	100	42	115	40 duplicate
	103 [648; Ethylamine (2TMS	71	63	-0.264	-0.436	15.410	0.418	101	41	99	43	55	114 duplicate
9223	103 [648; Ethylamine (2TMS	124	58	-0.266	-0.414	29.673	0.355	102	40	98	44	126	136 original
15569	103 [648; Ethylamine (2TMS	49	63	-0.269	-0.278	27.676	0.397	103	39	93	49	120	120 duplicate
18522	103 [648; Ethylamine (2TMS	89	34	-0.269	-0.640	22.259	0.571	104	38	114	28	93	18 duplicate
15215	103 [648; Ethylamine (2TMS	45	60	-0.278	-0.333	27.699	0.428	105	37	94	48	121	111 duplicate
13105	103 [648; Ethylamine (2TMS	25	48	-0.284	-0.634	25.171	0.479	106	36	113	29	107	77 duplicate

9229	103 [648; Ethylamine (2TMS 130 Trehalose	62 -0.285	-0.470	27.431	0.415	107	35	101	41	119	116 original
17703	103 [648; Ethylamine (2TMS 75 Lysine	63 -0.292	-0.608	37.245	0.442	108	34	110	32	139	101 duplicate
17220	103 [648; Ethylamine (2TMS 68 [570; Hypoxanthine (2TMS)]	63 -0.305	-0.774	16.100	0.598	109	33	137	5	62	10 duplicate
16688	103 [648; Ethylamine (2TMS 61 [NA]	63 -0.312	-0.345	15.645	0.431	110	32	95	47	58	108 duplicate
18945	103 [648; Ethylamine (2TMS 98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	47 -0.358	-0.704	28.458	0.547	111	31	126	16	117	31 duplicate
14315	103 [648; Ethylamine (2TMS 36 [596; N-Acetylglutamic acid (2TMS)]	63 -0.368	-0.722	28.659	0.480	112	30	131	11	125	75 duplicate
10184	103 [648; Ethylamine (2TMS 2 Serine	61 -0.368	-0.699	25.880	0.471	113	29	123	19	113	83 duplicate
12872	103 [648; Ethylamine (2TMS 23 Homoserine	63 -0.378	-0.705	21.151	0.511	114	28	127	15	87	55 duplicate
10864	103 [648; Ethylamine (2TMS 7 Threonine	63 -0.398	-0.643	28.439	0.434	115	27	116	28	124	108 duplicate
9207	103 [648; Ethylamine (2TMS 108 Octadecanoic acid	63 -0.399	-0.559	18.144	0.395	116	26	108	34	72	121 original
10997	103 [648; Ethylamine (2TMS 8 Isoleucine	54 -0.405	-0.648	24.192	0.435	117	25	117	25	108	105 duplicate
17073	103 [648; Ethylamine (2TMS 66 Glycine acid-3-phosphate	63 -0.428	-0.744	17.634	0.503	118	24	134	8	70	65 duplicate
15497	103 [648; Ethylamine (2TMS 48 Asparagine	63 -0.435	-0.617	21.763	0.519	119	23	112	30	89	48 duplicate
14104	103 [648; Ethylamine (2TMS 34 Aspartic acid	63 -0.439	-0.550	31.787	0.487	120	22	105	37	133	84 duplicate
15770	103 [648; Ethylamine (2TMS 51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	43 -0.449	-0.672	22.572	0.504	121	21	120	22	97	63 duplicate
13997	103 [648; Ethylamine (2TMS 33 Methionine	63 -0.461	-0.584	20.608	0.456	122	20	109	33	84	95 duplicate
13780	103 [648; Ethylamine (2TMS 31 [622; Parabanic acid (2TMS)]	63 -0.466	-0.699	20.962	0.474	123	19	124	18	85	82 duplicate
10595	103 [648; Ethylamine (2TMS 5 Leucine	44 -0.467	-0.617	14.535	0.525	124	18	111	31	46	42 duplicate
11129	103 [648; Ethylamine (2TMS 9 Proline	62 -0.479	-0.709	31.676	0.464	125	17	128	14	132	89 duplicate
16608	103 [648; Ethylamine (2TMS 60 Glycerol-3-phosphate	63 -0.483	-0.703	22.135	0.500	126	16	125	17	91	68 duplicate
9230	103 [648; Ethylamine (2TMS 131 [626; 5-Methylthioadenosine (3TMS)]	54 -0.497	-0.530	23.079	0.516	127	15	104	38	104	49 original
14419	103 [648; Ethylamine (2TMS 37 Phenylalanine	63 -0.503	-0.716	22.465	0.463	128	14	129	13	95	91 duplicate
17147	103 [648; Ethylamine (2TMS 67 Citric acid	63 -0.504	-0.687	22.804	0.392	129	13	122	20	101	123 duplicate
18137	103 [648; Ethylamine (2TMS 82 Lysine	38 -0.505	-0.719	21.168	0.592	130	12	130	12	88	14 duplicate
16527	103 [648; Ethylamine (2TMS 59 Ornithine; Arginine	63 -0.507	-0.870	38.623	0.494	131	11	119	23	141	69 duplicate
16120	103 [648; Ethylamine (2TMS 55 [612; 4-Aminobutyric acid (2TBS)]	63 -0.508	-0.667	23.124	0.569	132	10	118	24	105	19 duplicate
17292	103 [648; Ethylamine (2TMS 69 Arginine	59 -0.508	-0.733	25.671	0.507	133	9	132	10	109	60 duplicate
13889	103 [648; Ethylamine (2TMS 32 [729; N,N-Dimethyllysine methyl ester]	62 -0.512	-0.769	27.704	0.523	134	8	138	4	122	43 duplicate
	103 [648; Ethylamine (2TMS [626; beta-[(5-methyl-2-thienyl)methyl]amino-										
17832	103 [648; Ethylamine (2TMS 77 benzeneacetic acid methyl ester]	61 -0.518	-0.739	32.202	0.482	135	7	133	9	134	74 duplicate
13670	103 [648; Ethylamine (2TMS 30 [815; Ethyl-3(2H)-thiophenone]	63 -0.520	-0.642	30.816	0.427	136	6	115	27	130	112 duplicate
10322	103 [648; Ethylamine (2TMS 3 Ethanolamine	61 -0.554	-0.768	22.205	0.564	137	5	136	6	92	24 duplicate
11260	103 [648; Ethylamine (2TMS 10 Glycine	63 -0.560	-0.789	22.979	0.565	138	4	139	3	103	22 duplicate
	103 [648; Ethylamine (2TMS [619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]										
12515	103 [648; Ethylamine (2TMS 81 Tyrosine	30 -0.595	-0.817	15.218	0.663	139	3	140	2	51	2 duplicate
18078	103 [648; Ethylamine (2TMS 42 Glutamic acid	63 -0.602	-0.852	34.898	0.624	140	2	141	1	137	5 duplicate
14924	103 [648; Ethylamine (2TMS 62 Glutamine	59 -0.615	-0.767	33.370	0.480	141	1	135	7	136	76 duplicate
17571	104 [795; Erythritol (4TMS)] 73 [708; Glucose methoxyamine (5TMS)]	56 0.606	0.803	7.087	0.570	1	141	2	140	13	14 duplicate
12395	104 [795; Erythritol (4TMS)] 19 Alanine (BP) (3TMS)	63 0.584	0.717	8.693	0.581	2	140	7	135	26	10 duplicate
9242	104 [795; Erythritol (4TMS)] 106 [733; Threitol (4TMS)]	61 0.573	0.810	6.698	0.632	3	138	1	141	8	2 original
9249	104 [795; Erythritol (4TMS)] 113 Galactose-6-phosphate	61 0.573	0.695	6.769	0.584	4	139	11	131	10	9 original
9250	104 [795; Erythritol (4TMS)] 114 Fructose-6-phosphate	52 0.557	0.703	6.917	0.577	5	137	10	132	11	11 original
9259	104 [795; Erythritol (4TMS)] 123 [945; Galactofuranose-6-phosphate (7TMS)]	63 0.554	0.735	8.135	0.568	6	136	4	138	21	16 original
17886	104 [795; Erythritol (4TMS)] 78 Mannose	61 0.540	0.732	8.367	0.509	7	135	5	137	22	49 duplicate
17958	104 [795; Erythritol (4TMS)] 79 Glucose	63 0.534	0.715	32.122	0.572	8	134	8	134	134	13 duplicate
17769	104 [795; Erythritol (4TMS)] 76 Fructose	63 0.501	0.723	22.183	0.538	9	133	6	136	114	34 duplicate
10731	104 [795; Erythritol (4TMS)] 6 Glyceral	63 0.495	0.710	39.411	0.581	10	132	9	133	140	22 duplicate
14826	104 [795; Erythritol (4TMS)] 41 [639; Proline (2TMS)]	63 0.477	0.586	11.226	0.520	11	131	20	122	43	44 duplicate
14726	104 [795; Erythritol (4TMS)] 40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	63 0.471	0.685	32.402	0.530	12	130	12	130	135	37 duplicate
9257	104 [795; Erythritol (4TMS)] 121 [657; Erythritol (4TMS)]	54 0.468	0.759	12.380	0.564	13	129	3	139	52	20 original
14211	104 [795; Erythritol (4TMS)] 35 Pyroglutamic acid	63 0.456	0.658	38.918	0.523	14	128	17	125	139	43 duplicate

9246	104 [795; Erythritol (4TMS)]	110 [715; Erythritol (4TMS)]	53 0.451	0.665	10.406	0.606	15	127	18	128	37	6 original
9253	104 [795; Erythritol (4TMS)]	117 [724; Glycerol (3TMS)]	55 0.448	0.682	6.687	0.529	16	126	13	129	7	38 original
9251	104 [795; Erythritol (4TMS)]	115 Glucose-6-phosphate	61 0.438	0.672	21.894	0.505	17	125	15	127	112	54 original
18196	104 [795; Erythritol (4TMS)]	83 Sorbitol	58 0.422	0.270	19.031	0.388	18	124	65	77	99	130 duplicate
18364	104 [795; Erythritol (4TMS)]	86 [783; D-Galactono-1,4-lactone (4TMS)]	60 0.412	0.677	18.336	0.570	19	123	14	128	94	15 duplicate
9258	104 [795; Erythritol (4TMS)]	122 [844; Erythritol (4TMS)]	51 0.410	0.574	14.873	0.549	20	122	21	121	72	30 original
9261	104 [795; Erythritol (4TMS)]	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	63 0.402	0.647	28.927	0.507	21	121	18	124	126	62 original
17364	104 [795; Erythritol (4TMS)]	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	56 0.378	0.551	15.807	0.473	22	120	25	117	80	92 duplicate
16923	104 [795; Erythritol (4TMS)]	64 [789; Tyramine (3TMS)]	62 0.365	0.445	6.075	0.442	23	119	42	100	3	65 duplicate
9269	104 [795; Erythritol (4TMS)]	133 [855; Squalene]	63 0.355	0.380	7.115	0.428	24	118	55	87	14	107 original
11901	104 [795; Erythritol (4TMS)]	15 Alanine	63 0.354	0.493	16.040	0.541	25	117	34	108	83	32 duplicate
18309	104 [795; Erythritol (4TMS)]	85 [529; Methylethylacetic acid (4TMS)]	48 0.346	0.519	5.436	0.483	26	116	29	113	2	63 duplicate
13448	104 [795; Erythritol (4TMS)]	28 Malic acid	63 0.346	0.488	7.648	0.467	27	115	35	107	17	71 duplicate
15120	104 [795; Erythritol (4TMS)]	44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	49 0.338	0.572	7.888	0.565	28	114	22	120	20	19 duplicate
12273	104 [795; Erythritol (4TMS)]	18 [590; 1-Acetyl-2-thiohydantoin]	63 0.326	0.484	6.442	0.438	29	113	38	106	5	100 duplicate
9262	104 [795; Erythritol (4TMS)]	126 [559; Erythritol (4TMS)]	44 0.319	0.564	7.662	0.551	30	112	23	119	18	27 original
11775	104 [795; Erythritol (4TMS)]	14 Fumaric acid	63 0.319	0.475	8.662	0.439	31	111	37	105	25	99 duplicate
12636	104 [795; Erythritol (4TMS)]	21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	63 0.311	0.440	14.482	0.416	32	110	44	98	70	112 duplicate
14625	104 [795; Erythritol (4TMS)]	39 [828; 1-Phenylethanol (1TMS)]	62 0.309	0.470	14.074	0.473	33	109	38	104	67	66 duplicate
13221	104 [795; Erythritol (4TMS)]	26 Citramalic acid	63 0.308	0.427	14.542	0.394	34	108	46	96	71	124 duplicate
16768	104 [795; Erythritol (4TMS)]	62 [812; D-Xylofuranose (4TMS)]	63 0.306	0.512	11.993	0.485	35	107	31	111	51	58 duplicate
14523	104 [795; Erythritol (4TMS)]	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	63 0.305	0.458	6.586	0.464	36	106	41	101	6	74 duplicate
17638	104 [795; Erythritol (4TMS)]	74 [912; Tetradecanoic acid (1TMS)]	63 0.295	0.535	8.639	0.503	37	105	28	118	24	55 duplicate
18019	104 [795; Erythritol (4TMS)]	80 [772; D-Glucose (5TMS)]	61 0.295	0.528	28.167	0.454	38	104	26	114	124	80 duplicate
16279	104 [795; Erythritol (4TMS)]	56 [828; Orotic acid (3TMS)]	63 0.287	0.510	10.389	0.549	39	103	32	110	36	28 duplicate
18471	104 [795; Erythritol (4TMS)]	88 Gluconic acid	63 0.276	0.381	10.635	0.568	40	102	54	88	38	17 duplicate
11648	104 [795; Erythritol (4TMS)]	13 Uracil	63 0.269	0.444	14.033	0.553	41	101	43	99	66	26 duplicate
9270	104 [795; Erythritol (4TMS)]	134 Isomaltose	63 0.267	0.503	22.419	0.555	42	100	33	109	117	24 original
18418	104 [795; Erythritol (4TMS)]	87 [945; beta-D-Glucopyranose (5TMS)]	62 0.266	0.554	32.706	0.472	43	99	24	118	136	67 duplicate
15311	104 [795; Erythritol (4TMS)]	46 Arabinose	63 0.259	0.528	15.143	0.547	44	97	27	115	75	31 duplicate
18029	104 [795; Erythritol (4TMS)]	100 [857; Mannitol (5TMS)]	63 0.259	0.342	7.718	0.370	45	98	59	83	19	133 duplicate
12980	104 [795; Erythritol (4TMS)]	24 [725; 2-Ketooctanoic acid (2TMS)]	63 0.257	0.469	28.658	0.567	46	96	39	103	129	18 duplicate
16999	104 [795; Erythritol (4TMS)]	65 [846; 3-Deoxyglucitol (5TMS)]	62 0.252	0.512	12.645	0.537	47	95	30	112	53	35 duplicate
16446	104 [795; Erythritol (4TMS)]	58 [636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	63 0.247	0.299	14.332	0.409	48	94	61	81	69	116 duplicate
11391	104 [795; Erythritol (4TMS)]	11 Succinic acid	63 0.245	0.408	6.753	0.435	49	93	51	91	8	103 duplicate
9245	104 [795; Erythritol (4TMS)]	109 Octadecanoic acid	63 0.244	0.590	19.367	0.484	50	92	19	123	104	60 original
12026	104 [795; Erythritol (4TMS)]	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	63 0.241	0.422	15.637	0.576	51	91	47	85	79	12 duplicate
9274	104 [795; Erythritol (4TMS)]	138 [674; Ergosterol (1TMS)]	45 0.240	0.375	14.967	0.397	52	90	56	86	73	121 original
15681	104 [795; Erythritol (4TMS)]	50 [746; Ribonic acid-1,4-lactone (3TMS)]	60 0.235	0.420	17.933	0.501	54	88	49	93	90	56 duplicate
19108	104 [795; Erythritol (4TMS)]	102 [904; Galactose methoxyamine (5TMS)]	63 0.231	0.327	7.008	0.366	55	87	60	82	12	135 duplicate
13560	104 [795; Erythritol (4TMS)]	29 Erythritol	63 0.230	0.384	6.149	0.461	56	86	53	89	4	75 duplicate
9266	104 [795; Erythritol (4TMS)]	130 Trehalose	62 0.224	0.277	28.025	0.403	57	85	64	78	123	118 original
12150	104 [795; Erythritol (4TMS)]	17 [700; 2-methyl-1,2-propanediol (2TMS)]	63 0.218	0.420	15.428	0.486	58	84	48	94	77	57 duplicate
14316	104 [795; Erythritol (4TMS)]	36 [596; N-Acetylglutamic acid (2TMS)]	63 0.216	0.296	26.641	0.424	59	83	62	80	121	109 duplicate
19146	104 [795; Erythritol (4TMS)]	103 [648; Ethylamine (2TMS)]	62 0.204	0.222	13.944	0.509	60	82	72	70	65	50 duplicate
9265	104 [795; Erythritol (4TMS)]	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	58 0.203	0.427	11.055	0.559	61	81	45	97	42	23 original
9256	104 [795; Erythritol (4TMS)]	120 [945; Uridine (3TMS)]	53 0.194	0.180	10.293	0.426	62	80	75	67	34	108 original
12755	104 [795; Erythritol (4TMS)]	22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	51 0.194	0.343	11.539	0.446	63	79	58	84	50	89 duplicate
17704	104 [795; Erythritol (4TMS)]	75 Lysine	63 0.192	0.238	37.823	0.417	64	78	68	74	136	111 duplicate

9248	104 [795; Erythritol (4TMS)]	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	62	0.176	0.266	15.976	0.447	65	77	66	76	82	87 original
9247	104 [795; Erythritol (4TMS)]	111 [593; Erythritol (4TMS)]	41	0.168	0.204	19.921	0.343	68	76	73	69	107	139 original
17434	104 [795; Erythritol (4TMS)]	71 [731; Erythrose (3TMS)]	63	0.155	0.231	10.735	0.378	67	75	70	72	39	132 duplicate
9268	104 [795; Erythritol (4TMS)]	132 [895; Isomaltose methoxyamine (8TMS)]	41	0.151	0.259	15.579	0.450	68	74	67	75	78	83 original
18768	104 [795; Erythritol (4TMS)]	94 Hexadecanoic acid	63	0.146	0.461	18.251	0.528	69	73	40	102	100	39 duplicate
9254	104 [795; Erythritol (4TMS)]	118 [928; Glucopyranose-6-phosphate (6TMS)]	57	0.145	0.235	9.334	0.396	70	72	69	73	31	122 original
11520	104 [795; Erythritol (4TMS)]	12 Glycic acid	62	0.137	0.288	10.983	0.384	71	71	63	79	41	131 duplicate
9252	104 [795; Erythritol (4TMS)]	116 [882; Pseudouridine (5TMS)]	30	0.136	0.115	10.103	0.392	72	70	79	63	33	128 original
18859	104 [795; Erythritol (4TMS)]	96 myo-Inositol	48	0.133	0.008	16.785	0.326	73	69	80	52	97	140 duplicate
9276	104 [795; Erythritol (4TMS)]	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	48	0.126	0.121	15.208	0.450	74	68	78	64	76	84 original
9271	104 [795; Erythritol (4TMS)]	135 [902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	63	0.125	0.191	10.868	0.391	75	67	74	68	40	128 original
19069	104 [795; Erythritol (4TMS)]	101 [832; Dopamine (4TMS)]	63	0.121	0.113	11.385	0.507	76	66	80	62	48	51 duplicate
9277	104 [795; Erythritol (4TMS)]	141 Lanosta-8,24-dien-3-beta-ol	60	0.096	0.099	13.831	0.442	77	65	81	61	64	93 original
16363	104 [795; Erythritol (4TMS)]	57 [757; 2-Desoxy-pentos-3-yose dimethoxyamine (2TMS)]	54	0.092	0.419	12.657	0.519	78	84	50	92	54	45 duplicate
17074	104 [795; Erythritol (4TMS)]	66 Glycic acid-3-phosphate	63	0.075	0.148	7.456	0.444	79	63	77	65	16	91 duplicate
9260	104 [795; Erythritol (4TMS)]	124 [734; 1-Monodecenoylethanol (1TMS)]	58	0.072	0.052	22.508	0.345	80	62	85	57	118	137 original
9273	104 [795; Erythritol (4TMS)]	137 Ergosterol	63	0.068	0.079	13.670	0.394	81	61	83	59	62	125 original
18624	104 [795; Erythritol (4TMS)]	91 [766; beta-D-Methylglucopyranoside (4TMS)]	63	0.061	-0.026	18.073	0.465	82	60	93	49	92	73 duplicate
10460	104 [795; Erythritol (4TMS)]	4 Phosphoric acid	51	0.053	0.080	31.030	0.357	83	59	82	60	131	136 duplicate
18673	104 [795; Erythritol (4TMS)]	92 [680; Glycerol-2-phosphate (4TMS)]	53	0.051	0.381	8.756	0.448	84	58	57	85	27	86 duplicate
9264	104 [795; Erythritol (4TMS)]	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	44	0.021	0.041	8.508	0.422	85	57	88	56	23	110 original
18988	104 [795; Erythritol (4TMS)]	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	40	0.000	0.159	11.421	0.446	86	56	76	68	47	88 duplicate
16035	104 [795; Erythritol (4TMS)]	54 [NA]	54	-0.001	0.226	12.900	0.456	87	55	71	71	56	78 duplicate
10185	104 [795; Erythritol (4TMS)]	2 Serine	61	-0.004	0.017	18.139	0.437	88	54	88	54	83	102 duplicate
10865	104 [795; Erythritol (4TMS)]	7 Threonine	63	-0.010	-0.011	28.520	0.442	89	53	91	51	125	94 duplicate
9263	104 [795; Erythritol (4TMS)]	127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	38	-0.010	-0.014	7.242	0.402	90	52	92	50	15	120 original
9272	104 [795; Erythritol (4TMS)]	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.044	0.052	4.700	0.263	91	51	84	58	1	141 original
18946	104 [795; Erythritol (4TMS)]	98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	47	-0.077	-0.234	17.574	0.484	92	50	103	39	88	62 duplicate
16609	104 [795; Erythritol (4TMS)]	60 Glycerol-3-phosphate	63	-0.080	-0.131	20.154	0.512	93	49	96	46	108	47 duplicate
17148	104 [795; Erythritol (4TMS)]	67 Citric acid	63	-0.081	-0.118	22.245	0.449	94	48	95	47	115	85 duplicate
9275	104 [795; Erythritol (4TMS)]	139 [700; Ergosta-5,7-dien-3-ol]	37	-0.084	-0.275	17.463	0.345	95	47	108	34	87	138 original
11130	104 [795; Erythritol (4TMS)]	9 Proline	62	-0.094	0.010	26.643	0.433	96	46	89	53	122	105 duplicate
13781	104 [795; Erythritol (4TMS)]	31 [622; Parabanic acid (2TMS)]	63	-0.102	-0.136	11.458	0.403	97	45	97	45	48	119 duplicate
13335	104 [795; Erythritol (4TMS)]	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	52	-0.121	-0.381	19.320	0.454	98	44	119	23	103	81 duplicate
18903	104 [795; Erythritol (4TMS)]	97 [756; beta-D-Methylglucopyranoside (4TMS)]	51	-0.126	-0.036	19.753	0.539	99	43	94	48	105	33 duplicate
17503	104 [795; Erythritol (4TMS)]	72 [919; D-Xylopyranose (4TMS)]	62	-0.130	-0.197	11.235	0.391	100	42	100	42	44	127 duplicate
10323	104 [795; Erythritol (4TMS)]	3 Ethanolamine	61	-0.158	-0.322	12.681	0.611	101	41	114	28	55	5 duplicate
12873	104 [795; Erythritol (4TMS)]	23 Homoserine	63	-0.163	-0.355	13.080	0.433	102	40	118	24	58	104 duplicate
9241	104 [795; Erythritol (4TMS)]	105 [705; 2-Ketogluconic acid (5TMS)]	47	-0.177	-0.201	12.938	0.531	103	39	101	41	57	36 original
9244	104 [795; Erythritol (4TMS)]	108 Octadecenoic acid	63	-0.178	-0.172	9.252	0.437	104	37	98	44	30	101 original
9243	104 [795; Erythritol (4TMS)]	107 9-(Z)-Octadecenoic acid	63	-0.178	-0.295	13.811	0.396	105	38	111	31	63	123 original
16528	104 [795; Erythritol (4TMS)]	59 Ornithine; Arginine	63	-0.183	-0.173	38.489	0.410	106	36	98	43	141	115 duplicate
14420	104 [795; Erythritol (4TMS)]	37 Phenylalanine	63	-0.184	-0.254	21.446	0.457	107	35	106	36	111	77 duplicate
15948	104 [795; Erythritol (4TMS)]	53 Glycerol-2-phosphate	63	-0.185	-0.203	11.484	0.390	108	34	102	40	49	129 duplicate
13890	104 [795; Erythritol (4TMS)]	32 [728; N,N-Dimethyllysine methyl ester]	62	-0.180	-0.262	17.307	0.487	109	33	107	35	86	59 duplicate
13106	104 [795; Erythritol (4TMS)]	25 [709; 2,5-Diaminovalerolactam (2TMS)]	47	-0.191	-0.253	16.540	0.470	110	32	105	37	84	69 duplicate
10998	104 [795; Erythritol (4TMS)]	8 Isoleucine	55	-0.196	0.026	17.884	0.404	111	31	87	55	89	117 duplicate
15405	104 [795; Erythritol (4TMS)]	47 [NA]	63	-0.201	-0.242	13.136	0.450	112	30	104	38	59	82 duplicate



15023	104 [795; Erythritol (4TMS)]	43	[548; Leucine (2TBS)]	59	-0.202	-0.337	9.422	0.524	113	29	118	26	32	42 duplicate
9255	104 [795; Erythritol (4TMS)]	119	[931; myo-Inositol-2-phosphate (7TMS)]	63	-0.212	-0.314	10.389	0.432	114	28	113	29	35	108 original
18574	104 [795; Erythritol (4TMS)]	90	[910; 9-(Z)-Hexadecanoic acid (1TMS)]	63	-0.233	-0.324	9.027	0.440	115	27	115	27	29	96 duplicate
18079	104 [795; Erythritol (4TMS)]	81	Tyrosine	63	-0.244	-0.313	33.280	0.871	116	26	112	30	137	1 duplicate
11261	104 [795; Erythritol (4TMS)]	10	Glycine	63	-0.256	-0.479	18.270	0.554	117	25	127	15	101	25 duplicate
18253	104 [795; Erythritol (4TMS)]	84	Mannitol	61	-0.288	-0.389	31.055	0.467	118	24	120	22	132	72 duplicate
17833	104 [795; Erythritol (4TMS)]	77	[826; beta-[(5-methyl-2-thenyl)methyl]eneamino-benzenecarboxylic acid methyl ester]	61	-0.284	-0.291	29.471	0.471	119	23	110	32	128	68 duplicate
14925	104 [795; Erythritol (4TMS)]	52	Glutamic acid	60	-0.289	-0.276	28.742	0.414	120	22	109	33	130	114 duplicate
15771	104 [795; Erythritol (4TMS)]	41	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.292	-0.391	18.630	0.458	121	21	122	20	86	76 duplicate
13998	104 [795; Erythritol (4TMS)]	33	Methionine	63	-0.294	-0.471	13.278	0.445	122	20	125	17	60	80 duplicate
14105	104 [795; Erythritol (4TMS)]	34	Aspartic acid	63	-0.301	-0.390	31.928	0.414	123	19	121	21	133	113 duplicate
13671	104 [795; Erythritol (4TMS)]	30	[915; Ethyl-3-(2H)-thiophenone]	63	-0.310	-0.344	29.396	0.441	124	18	117	25	127	95 duplicate
18721	104 [795; Erythritol (4TMS)]	93	[607; Putrescine (4TMS)]	59	-0.314	-0.410	18.004	0.468	125	17	123	19	91	70 duplicate
9267	104 [795; Erythritol (4TMS)]	131	[626; 5-Methylthioadenosine (3TMS)]	54	-0.317	-0.557	16.951	0.517	126	16	130	12	85	46 original
15498	104 [795; Erythritol (4TMS)]	48	Asparagine	63	-0.343	-0.557	15.109	0.510	127	15	129	13	74	48 duplicate
17293	104 [795; Erythritol (4TMS)]	69	Arginine	60	-0.356	-0.472	21.967	0.484	128	14	126	16	113	61 duplicate
16689	104 [795; Erythritol (4TMS)]	61	[NA]	63	-0.365	-0.525	8.855	0.439	129	13	128	14	28	98 duplicate
15216	104 [795; Erythritol (4TMS)]	45	Homocysteine	60	-0.391	-0.639	21.252	0.439	130	12	131	11	110	97 duplicate
17221	104 [795; Erythritol (4TMS)]	68	[570; Hypoxanthine (2TMS)]	20	-0.411	-0.708	13.454	0.528	131	11	135	7	61	40 duplicate
12516	104 [795; Erythritol (4TMS)]	20	[619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.428	-0.861	15.818	0.624	132	10	140	2	81	3 duplicate
15590	104 [795; Erythritol (4TMS)]	49	[877; Pyrophosphoric acid (4TMS)]	63	-0.437	-0.646	22.396	0.455	133	9	133	9	116	79 duplicate
10046	104 [795; Erythritol (4TMS)]	1	[938; Sulfuric acid (2TMS)]	35	-0.449	-0.450	11.357	0.476	134	8	124	18	45	64 duplicate
18814	104 [795; Erythritol (4TMS)]	95	[770; 3,4,6-Tris(hydroxyphenyl)ethanolamine (5TMS)]	49	-0.463	-0.680	18.834	0.549	135	7	134	8	98	29 duplicate
16846	104 [795; Erythritol (4TMS)]	63	Glutamine	51	-0.506	-0.641	19.315	0.506	136	6	132	10	102	53 duplicate
16121	104 [795; Erythritol (4TMS)]	55	[612; 4-Aminobutyric acid (2TBS)]	43	-0.524	-0.763	22.816	0.602	137	5	137	5	119	7 duplicate
15860	104 [795; Erythritol (4TMS)]	52	[NA]	45	-0.533	-0.730	20.757	0.561	138	4	138	6	109	21 duplicate
10598	104 [795; Erythritol (4TMS)]	5	Leucine	45	-0.590	-0.766	14.137	0.525	139	3	138	4	69	41 duplicate
18138	104 [795; Erythritol (4TMS)]	82	Lysine	39	-0.641	-0.904	19.784	0.619	140	2	141	1	108	4 duplicate
18523	104 [795; Erythritol (4TMS)]	89	[775; Dopamine (4TMS)]	35	-0.681	-0.856	18.561	0.596	141	1	139	3	95	8 duplicate
19147	105 [705; 2-Ketogluconic acid	103	[648; Ethylamine (2TMS)]	48	0.817	0.954	4.669	0.676	1	141	1	141	1	1 duplicate
18674	105 [705; 2-Ketogluconic acid	92	[680; Glycerol-2-phosphate (4TMS)]	48	0.762	0.896	8.914	0.534	2	140	4	138	13	50 duplicate
18904	105 [705; 2-Ketogluconic acid	97	[756; beta-D-Methylglucopyranoside (4TMS)]	48	0.754	0.911	12.201	0.585	3	139	2	140	41	27 duplicate
9306	105 [705; 2-Ketogluconic acid	134	Isomaltose	48	0.707	0.896	18.888	0.658	4	138	3	139	92	3 original
11649	105 [705; 2-Ketogluconic acid	13	Uracil	48	0.674	0.895	10.963	0.639	5	136	5	137	31	8 duplicate
18070	105 [705; 2-Ketogluconic acid	101	[832; Dopamine (4TMS)]	48	0.674	0.873	5.594	0.587	6	137	10	132	2	28 duplicate
18722	105 [705; 2-Ketogluconic acid	93	[607; Putrescine (4TMS)]	46	0.666	0.771	17.058	0.414	7	135	28	114	82	110 duplicate
16384	105 [705; 2-Ketogluconic acid	57	[757; 2-Deoxy-pentose-3-yose dimethoxyamine (2TMS)]	48	0.649	0.884	6.395	0.631	8	134	6	136	6	10 duplicate
17000	105 [705; 2-Ketogluconic acid	55	[646; 3-Deoxyglucitol (5TMS)]	48	0.645	0.854	6.077	0.632	9	133	14	128	5	9 duplicate
16280	105 [705; 2-Ketogluconic acid	56	[828; Oxalic acid (3TMS)]	48	0.644	0.863	7.078	0.625	10	132	7	135	8	14 duplicate
9301	105 [705; 2-Ketogluconic acid	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	48	0.631	0.857	5.940	0.616	11	131	13	129	4	16 original
15312	105 [705; 2-Ketogluconic acid	46	Arabinose	48	0.622	0.879	10.867	0.623	12	130	8	134	27	15 duplicate
18989	105 [705; 2-Ketogluconic acid	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	36	0.619	0.835	12.319	0.602	13	129	17	125	44	21 duplicate
12027	105 [705; 2-Ketogluconic acid	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	48	0.619	0.879	12.789	0.629	14	128	9	133	50	12 duplicate
14626	105 [705; 2-Ketogluconic acid	39	[828; 1-Phenylethanol (1TMS)]	48	0.594	0.853	9.690	0.568	15	126	15	127	19	33 duplicate
18825	105 [705; 2-Ketogluconic acid	91	[766; beta-D-Methylglucopyranoside (4TMS)]	48	0.594	0.800	9.021	0.505	16	127	23	119	14	67 duplicate
18472	105 [705; 2-Ketogluconic acid	88	Gluconic acid	48	0.589	0.739	8.656	0.612	17	125	30	112	12	17 duplicate
12991	105 [705; 2-Ketogluconic acid	24	[725; 2-Ketooctanoic acid (2TMS)]	48	0.587	0.873	24.990	0.658	18	124	11	131	122	2 duplicate

13561	105 [705; 2-Ketogluconic acid	29	Erythritol	48	0.574	0.838	10,191	0.585	19	123	16	126	23	28 duplicate
15682	105 [705; 2-Ketogluconic acid	50	[746; Ribonic acid-1,4-lactone (3TMS)]	48	0.568	0.859	18,931	0.567	20	122	12	130	93	35 duplicate
9300	105 [705; 2-Ketogluconic acid	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	44	0.564	0.824	6,459	0.528	21	121	19	123	7	57 original
12151	105 [705; 2-Ketogluconic acid	17	[700; 2-methyl-1,2-propanediol (2TMS)]	48	0.559	0.804	12,949	0.561	22	120	22	120	52	40 duplicate
16947	105 [705; 2-Ketogluconic acid	63	Glutamine	38	0.556	0.821	19,382	0.579	23	119	20	122	97	31 duplicate
16036	105 [705; 2-Ketogluconic acid	54	[NA]	48	0.534	0.792	11,212	0.559	24	118	25	117	33	42 duplicate
18365	105 [705; 2-Ketogluconic acid	86	[793; D-Galactono-1,4-lactone (4TMS)]	45	0.507	0.834	15,805	0.643	25	117	18	124	72	5 duplicate
11521	105 [705; 2-Ketogluconic acid	12	Glyceric acid	48	0.493	0.773	13,851	0.536	26	116	26	116	63	49 duplicate
15661	105 [705; 2-Ketogluconic acid	52	[NA]	30	0.490	0.794	25,094	0.593	27	115	24	118	123	24 duplicate
14524	105 [705; 2-Ketogluconic acid	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	48	0.484	0.820	8,490	0.604	28	114	21	121	11	19 duplicate
18310	105 [705; 2-Ketogluconic acid	85	[528; Methylcitric acid (4TMS)]	32	0.452	0.630	5,935	0.509	29	113	38	104	3	64 duplicate
18254	105 [705; 2-Ketogluconic acid	84	Mannitol	46	0.447	0.773	21,577	0.516	30	112	27	115	109	61 duplicate
11392	105 [705; 2-Ketogluconic acid	11	Succinic acid	48	0.447	0.673	9,578	0.531	31	111	34	108	17	53 duplicate
16769	105 [705; 2-Ketogluconic acid	62	[812; D-Xylofuranose (4TMS)]	48	0.441	0.690	11,779	0.603	32	110	33	109	39	20 duplicate
12756	105 [705; 2-Ketogluconic acid	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	42	0.440	0.756	12,228	0.567	33	109	29	113	42	36 duplicate
9289	105 [705; 2-Ketogluconic acid	127	[777; Fructose-6-phosphate methoxyamine (5TMS)]	39	0.436	0.654	9,516	0.429	34	108	38	108	16	104 original
18524	105 [705; 2-Ketogluconic acid	89	[775; Dopamine (4TMS)]	19	0.380	0.713	17,746	0.511	35	107	31	111	84	62 duplicate
11776	105 [705; 2-Ketogluconic acid	14	Fumaric acid	48	0.356	0.710	12,735	0.559	36	106	32	110	49	41 duplicate
10047	105 [705; 2-Ketogluconic acid	1	[938; Sulfuric acid (2TMS)]	35	0.351	0.598	10,884	0.481	38	104	40	102	28	76 duplicate
9282	105 [705; 2-Ketogluconic acid	110	[715; Erythritol (4TMS)]	48	0.337	0.508	11,583	0.642	39	103	43	99	37	7 original
17365	105 [705; 2-Ketogluconic acid	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	42	0.334	0.130	16,265	0.361	40	102	72	70	77	39 duplicate
18575	105 [705; 2-Ketogluconic acid	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	48	0.333	0.469	10,534	0.377	41	100	52	90	24	128 duplicate
17222	105 [705; 2-Ketogluconic acid	68	[570; Hypoxanthine (2TMS)]	7	0.333	0.201	15,382	0.084	42	101	69	73	70	141 duplicate
19030	105 [705; 2-Ketogluconic acid	100	[857; Mannitol (5TMS)]	48	0.316	0.626	9,447	0.498	43	99	39	103	15	70 duplicate
9289	105 [705; 2-Ketogluconic acid	117	[724; Glycerol (3TMS)]	46	0.304	0.482	10,615	0.504	44	98	48	94	25	68 original
9294	105 [705; 2-Ketogluconic acid	122	[644; Erythritol (4TMS)]	48	0.303	0.593	15,950	0.530	45	97	41	101	73	55 original
9278	105 [705; 2-Ketogluconic acid	106	[733; Threitol (4TMS)]	48	0.299	0.459	9,793	0.595	46	96	54	88	20	23 original
9291	105 [705; 2-Ketogluconic acid	119	[931; myo-Inositol-2-phosphate (7TMS)]	48	0.298	0.473	10,777	0.439	47	95	51	91	26	94 original
15121	105 [705; 2-Ketogluconic acid	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	48	0.294	0.495	10,134	0.543	48	94	44	88	22	45 duplicate
13449	105 [705; 2-Ketogluconic acid	28	Malic acid	48	0.287	0.667	9,637	0.539	49	93	35	107	18	48 duplicate
13222	105 [705; 2-Ketogluconic acid	26	Citramalic acid	48	0.278	0.481	13,055	0.508	50	91	49	93	55	65 duplicate
9307	105 [705; 2-Ketogluconic acid	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	48	0.278	0.465	11,050	0.475	51	92	53	89	32	78 original	
15406	105 [705; 2-Ketogluconic acid	47	[NA]	48	0.270	0.351	11,569	0.520	52	90	61	81	36	59 duplicate
12637	105 [705; 2-Ketogluconic acid	21	[878; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	48	0.266	0.458	13,078	0.507	53	89	55	87	57	68 duplicate
9284	105 [705; 2-Ketogluconic acid	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	47	0.254	0.454	19,772	0.430	54	88	56	86	98	103 original
17770	105 [705; 2-Ketogluconic acid	76	Fructose	48	0.252	0.496	21,542	0.582	55	87	47	95	108	29 duplicate
9293	105 [705; 2-Ketogluconic acid	121	[657; Erythritol (4TMS)]	46	0.239	0.344	16,412	0.471	56	86	63	79	78	81 original
9287	105 [705; 2-Ketogluconic acid	115	Glucose-6-phosphate	47	0.234	0.384	20,235	0.630	57	85	58	84	101	11 original
17897	105 [705; 2-Ketogluconic acid	78	Mannose	46	0.229	0.376	10,942	0.581	58	84	59	83	30	30 duplicate
9292	105 [705; 2-Ketogluconic acid	120	[945; Uridine (3TMS)]	45	0.224	0.182	11,516	0.511	59	83	71	71	35	63 original
14727	105 [705; 2-Ketogluconic acid	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	48	0.218	0.487	26,413	0.497	60	81	46	96	131	71 duplicate
19109	105 [705; 2-Ketogluconic acid	102	[904; Galactose methoxyamine (5TMS)]	48	0.218	0.476	11,968	0.487	61	82	50	92	40	74 duplicate
17572	105 [705; 2-Ketogluconic acid	73	[708; Glucose methoxyamine (5TMS)]	41	0.210	0.222	10,890	0.472	62	80	67	75	29	80 duplicate
9279	105 [705; 2-Ketogluconic acid	107	9-(Z)-Octadecenoic acid	48	0.200	0.188	11,740	0.407	63	79	70	72	38	114 original
9298	105 [705; 2-Ketogluconic acid	128	[559; Erythritol (4TMS)]	45	0.190	0.349	13,091	0.529	64	78	62	80	58	56 original
18419	105 [705; 2-Ketogluconic acid	87	[945; beta-D-Glucopyranose (5TMS)]	46	0.173	0.341	30,524	0.597	65	77	64	78	137	22 duplicate
18815	105 [705; 2-Ketogluconic acid	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	34	0.169	-0.025	23,413	0.457	66	76	82	60	114	86 duplicate
15949	105 [705; 2-Ketogluconic acid	53	Glycerol-2-phosphate	48	0.138	0.284	15,960	0.379	67	75	68	76	74	123 duplicate
9313	105 [705; 2-Ketogluconic acid	141	Lanosta-8,24-dien-3-beta-ol	45	0.135	0.317	16,748	0.462	68	74	65	77	80	84 original
14212	105 [705; 2-Ketogluconic acid	35	Pyroglutamic acid	48	0.124	0.354	33,530	0.542	69	73	80	82	140	47 duplicate

9312	105 [705; 2-Ketogluconic acid 140 [992; Ergosta-7,22-dien-3-ol (1TMS)]	33	0.114	0.401	16,661	0.388	70	72	57	85	79	119 original
12274	105 [705; 2-Ketogluconic acid 18 [590; 1-Acetyl-2-thiohydantoin]	48	0.071	0.085	11,264	0.395	71	71	73	69	34	116 duplicate
9304	105 [705; 2-Ketogluconic acid 132 [895; Isomaltose methoxyamine (8TMS)]	38	0.058	0.651	14,764	0.471	72	70	70	105	68	82 original
9288	105 [705; 2-Ketogluconic acid 116 [882; Pseudouridine (5TMS)]	20	0.053	0.584	7,618	0.435	73	69	42	100	9	88 original
17639	105 [705; 2-Ketogluconic acid 74 [912; Tetradecanoic acid (1TMS)]	48	0.051	0.212	13,495	0.463	74	68	68	74	61	83 duplicate
18769	105 [705; 2-Ketogluconic acid 94 Hexadecanoic acid	48	0.007	0.022	17,793	0.477	75	67	76	66	85	77 duplicate
9287	105 [705; 2-Ketogluconic acid 125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	48	0.000	0.011	27,862	0.526	76	66	79	83	135	58 original
9283	105 [705; 2-Ketogluconic acid 111 [583; Erythritol (4TMS)]	36	-0.006	0.011	23,177	0.308	77	65	78	64	111	138 original
9281	105 [705; 2-Ketogluconic acid 109 Octadecanoic acid	48	-0.011	0.018	20,050	0.453	78	64	77	65	100	89 original
9309	105 [705; 2-Ketogluconic acid 137 Ergosterol	48	-0.023	-0.157	15,025	0.417	79	63	87	55	68	109 original
18020	105 [705; 2-Ketogluconic acid 80 [772; D-Glucose (5TMS)]	48	-0.043	-0.008	26,618	0.562	80	62	80	62	132	38 duplicate
9311	105 [705; 2-Ketogluconic acid 139 [700; Ergosta-5,7-dien-3-ol]	26	-0.046	0.038	20,318	0.327	81	61	75	67	103	137 original
17504	105 [705; 2-Ketogluconic acid 72 [919; D-Xylopyranose (4TMS)]	47	-0.056	-0.072	14,745	0.377	82	60	84	58	65	124 duplicate
10732	105 [705; 2-Ketogluconic acid 6 Glycerol	48	-0.066	-0.073	33,851	0.566	83	59	85	57	141	37 duplicate
16690	105 [705; 2-Ketogluconic acid 61 [NA]	48	-0.073	0.040	12,434	0.449	84	58	74	68	46	92 duplicate
15591	105 [705; 2-Ketogluconic acid 49 [877; Pyrophosphoric acid (4TMS)]	48	-0.074	-0.043	25,127	0.434	85	57	83	59	124	98 duplicate
18197	105 [705; 2-Ketogluconic acid 83 Sorbitol	42	-0.082	-0.434	19,333	0.386	86	56	104	38	96	118 duplicate
15024	105 [705; 2-Ketogluconic acid 43 [548; Leucine (2TBS)]	44	-0.085	-0.204	12,438	0.344	87	55	92	50	47	134 duplicate
9286	105 [705; 2-Ketogluconic acid 124 [734; 1-Monodeoxyglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	43	-0.092	-0.210	26,774	0.408	88	54	93	49	133	113 original
18860	105 [705; 2-Ketogluconic acid 96 myo-Inositol	33	-0.098	-0.018	19,793	0.222	89	53	81	61	99	140 duplicate
9308	105 [705; 2-Ketogluconic acid 136 [748; D-Scdheptulose-7-phosphate (7TMS)]	17	-0.103	-0.174	7,891	0.279	90	52	88	54	10	139 original
14827	105 [705; 2-Ketogluconic acid 41 [839; Proline (2TMS)]	48	-0.144	-0.197	13,605	0.460	91	51	89	53	62	85 duplicate
9285	105 [705; 2-Ketogluconic acid 113 Galactose-6-phosphate	47	-0.145	-0.106	12,455	0.593	92	50	86	56	48	25 original
12396	105 [705; 2-Ketogluconic acid 19 Alanine (BP) (3TMS)	48	-0.158	-0.204	13,202	0.543	93	49	91	51	59	46 duplicate
9305	105 [705; 2-Ketogluconic acid 133 [855; Squalene]	48	-0.168	-0.231	14,430	0.411	94	48	97	45	64	112 original
15217	105 [705; 2-Ketogluconic acid 45 Homocysteine	45	-0.172	-0.331	25,144	0.349	95	47	94	48	125	133 duplicate
19184	105 [705; 2-Ketogluconic acid 104 [795; Erythritol (4TMS)]	47	-0.177	-0.201	12,938	0.531	96	46	90	52	51	52 duplicate
17435	105 [705; 2-Ketogluconic acid 71 [731; Erythrose (3TMS)]	48	-0.186	-0.321	12,266	0.438	97	45	96	46	43	95 duplicate
9290	105 [705; 2-Ketogluconic acid 118 [928; Glucopyranose-6-phosphate (6TMS)]	48	-0.215	-0.332	14,799	0.432	98	44	98	44	67	100 original
9280	105 [705; 2-Ketogluconic acid 108 Octadecenoic acid	47	-0.214	-0.418	15,365	0.431	99	43	102	40	69	102 original
13107	105 [705; 2-Ketogluconic acid 25 [709; 2,5-Diaminovalerolactam (2TMS)]	45	-0.238	-0.721	23,857	0.517	100	42	126	16	117	60 duplicate
15499	105 [705; 2-Ketogluconic acid 48 Asparagine	48	-0.257	-0.396	16,247	0.533	101	41	101	41	76	51 duplicate
9303	105 [705; 2-Ketogluconic acid 131 [626; 5-Methylthioadenosine (3TMS)]	41	-0.271	-0.272	20,867	0.568	102	40	95	47	107	34 original
9286	105 [705; 2-Ketogluconic acid 114 Fructose-6-phosphate	40	-0.285	-0.353	13,315	0.576	103	39	100	42	60	32 original
17149	105 [705; 2-Ketogluconic acid 67 Citric acid	48	-0.298	-0.489	17,949	0.365	104	38	105	37	87	130 duplicate
9295	105 [705; 2-Ketogluconic acid 123 [945; Galactotriuranose-6-phosphate (7TMS)]	48	-0.312	-0.568	13,037	0.551	105	37	108	34	54	43 original
9310	105 [705; 2-Ketogluconic acid 138 [674; Ergosterol (1TMS)]	32	-0.327	-0.341	20,241	0.418	106	36	99	43	102	107 original
16610	105 [705; 2-Ketogluconic acid 60 Glycerol-3-phosphate	48	-0.362	-0.544	16,831	0.494	107	35	106	36	81	73 duplicate
16122	105 [705; 2-Ketogluconic acid 55 [812; 4-Aminobutyric acid (2TBS)]	27	-0.385	-0.419	20,352	0.531	108	34	103	39	104	54 duplicate
18139	105 [705; 2-Ketogluconic acid 82 Lysine	23	-0.407	-0.601	9,963	0.483	109	33	112	30	21	75 duplicate
16924	105 [705; 2-Ketogluconic acid 64 [789; Tyramine (3TMS)]	48	-0.422	-0.577	12,971	0.456	110	32	109	33	53	87 duplicate
17834	105 [705; 2-Ketogluconic acid [826; beta-[[[5-methyl-2-thenyl]methyleneamino- benzeneacetic acid methyl ester]	46	-0.432	-0.689	23,324	0.382	111	31	120	22	112	122 duplicate
14421	105 [705; 2-Ketogluconic acid 37 Phenylalanine	48	-0.438	-0.682	17,739	0.418	112	30	119	23	83	108 duplicate
15772	105 [705; 2-Ketogluconic acid 51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	28	-0.439	-0.695	20,369	0.395	113	29	121	21	105	117 duplicate
14106	105 [705; 2-Ketogluconic acid 34 Aspartic acid	48	-0.441	-0.546	25,464	0.383	114	28	107	35	126	120 duplicate
12874	105 [705; 2-Ketogluconic acid 23 Homoserine	48	-0.443	-0.714	18,275	0.452	115	27	123	19	89	90 duplicate
10324	105 [705; 2-Ketogluconic acid 3 Ethanolamine	46	-0.453	-0.642	19,132	0.551	116	26	114	28	95	44 duplicate
13336	105 [705; 2-Ketogluconic acid 27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	37	-0.456	-0.737	24,655	0.432	117	25	130	12	121	101 duplicate
18947	105 [705; 2-Ketogluconic acid 98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	34	-0.465	-0.722	24,619	0.451	118	24	127	15	120	91 duplicate

9302	105 [705; 2-Ketogluconic acid 130	Trehalose	48	-0.473	-0.628	23.374	0.403	119	22	113	29	113	115 original
14317	105 [705; 2-Ketogluconic acid 36	[596; N-Acetylglutamic acid (2TMS)]	48	-0.473	-0.726	23.524	0.437	120	23	128	14	116	97 duplicate
13999	105 [705; 2-Ketogluconic acid 33	Methionine	48	-0.475	-0.596	18.022	0.342	121	21	111	31	88	135 duplicate
10461	105 [705; 2-Ketogluconic acid 4	Phosphoric acid	36	-0.486	-0.584	27.851	0.382	122	19	110	32	134	121 duplicate
12517	105 [705; 2-Ketogluconic acid 20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	15	-0.486	-0.759	12.348	0.498	123	20	134	8	45	69 duplicate
16529	105 [705; 2-Ketogluconic acid 59	Omithine; Arginine	48	-0.491	-0.644	31.302	0.374	124	17	115	27	138	127 duplicate
10866	105 [705; 2-Ketogluconic acid 7	Threonine	48	-0.491	-0.682	23.443	0.349	125	18	118	24	115	132 duplicate
17294	105 [705; 2-Ketogluconic acid 69	Arginine	44	-0.495	-0.747	19.071	0.484	126	16	132	10	94	72 duplicate
10597	105 [705; 2-Ketogluconic acid 5	Leucine	29	-0.498	-0.718	13.063	0.424	127	15	125	17	56	105 duplicate
11262	105 [705; 2-Ketogluconic acid 10	Glycine	48	-0.498	-0.780	16.057	0.605	128	14	137	5	75	18 duplicate
13672	105 [705; 2-Ketogluconic acid 30	[815; Ethyl-3(2H)-thiophenone]	48	-0.520	-0.655	24.398	0.387	129	13	116	26	118	129 duplicate
10999	105 [705; 2-Ketogluconic acid 8	Isoleucine	39	-0.522	-0.668	20.631	0.332	130	12	117	25	106	138 duplicate
13782	105 [705; 2-Ketogluconic acid 31	[622; Parabanic acid (2TMS)]	48	-0.546	-0.716	18.886	0.418	131	11	124	18	91	108 duplicate
14928	105 [705; 2-Ketogluconic acid 42	Glutamic acid	44	-0.564	-0.777	25.820	0.368	132	10	135	7	128	128 duplicate
11902	105 [705; 2-Ketogluconic acid 15	Alanine	48	-0.571	-0.828	18.522	0.642	133	9	139	3	90	6 duplicate
17705	105 [705; 2-Ketogluconic acid 75	Lysine	48	-0.574	-0.734	31.498	0.438	134	8	129	13	139	86 duplicate
17859	105 [705; 2-Ketogluconic acid 79	Glucose	48	-0.589	-0.785	30.374	0.625	135	7	136	6	136	13 duplicate
16447	105 [705; 2-Ketogluconic acid 58	[636; 4R-Acetalamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	48	-0.590	-0.703	17.903	0.411	136	6	122	20	86	111 duplicate
13891	105 [705; 2-Ketogluconic acid 32	[729; N,N-Dimethyllysine methyl ester]	47	-0.593	-0.845	25.612	0.474	137	5	141	1	127	79 duplicate
11131	105 [705; 2-Ketogluconic acid 9	Proline	47	-0.604	-0.739	26.192	0.377	138	4	131	11	130	125 duplicate
17075	105 [705; 2-Ketogluconic acid 68	Glyceral acid-3-phosphate	48	-0.612	-0.802	15.568	0.440	139	3	138	4	71	93 duplicate
16080	105 [705; 2-Ketogluconic acid 81	Tyrosine	48	-0.613	-0.839	24.483	0.649	140	2	140	2	119	4 duplicate
10186	105 [705; 2-Ketogluconic acid 2	Serine	46	-0.633	-0.766	22.717	0.360	141	1	133	9	110	131 duplicate
9317	106 [733; Threitol (4TMS)]	110 [715; Erythritol (4TMS)]	52	0.802	0.980	9.825	0.731	1	141	1	141	30	1 original
9329	106 [733; Threitol (4TMS)]	122 [644; Erythritol (4TMS)]	50	0.889	0.965	15.677	0.728	2	140	2	140	71	2 original
9324	106 [733; Threitol (4TMS)]	117 [724; Glycerol (3TMS)]	55	0.857	0.944	6.847	0.690	3	139	5	137	4	16 original
9328	106 [733; Threitol (4TMS)]	121 [637; Erythritol (4TMS)]	53	0.837	0.955	14.854	0.678	4	138	4	138	67	22 original
15122	106 [733; Threitol (4TMS)]	49 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	44	0.835	0.957	4.817	0.698	5	137	3	139	1	11 duplicate
17771	106 [733; Threitol (4TMS)]	76 Fructose	62	0.803	0.934	18.318	0.684	6	136	6	136	86	19 duplicate
9333	106 [733; Threitol (4TMS)]	126 [559; Erythritol (4TMS)]	44	0.770	0.902	9.686	0.710	7	135	9	133	27	7 original
14728	106 [733; Threitol (4TMS)]	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	62	0.759	0.926	30.151	0.683	8	134	7	135	133	21 duplicate
17898	106 [733; Threitol (4TMS)]	78 Mannose	60	0.701	0.891	8.481	0.643	9	133	10	132	17	35 duplicate
9322	106 [733; Threitol (4TMS)]	115 Glucose-6-phosphate	61	0.686	0.889	18.924	0.626	10	132	11	131	88	42 original
14213	106 [733; Threitol (4TMS)]	35 Pyroglutamic acid	62	0.682	0.883	36.125	0.656	11	131	14	128	139	28 duplicate
17573	106 [733; Threitol (4TMS)]	73 [708; Glucose methoxyamine (5TMS)]	55	0.678	0.883	7.531	0.577	12	130	13	129	9	70 duplicate
18368	106 [733; Threitol (4TMS)]	86 [793; D-Galactono-1,4-lactone (4TMS)]	59	0.658	0.808	13.446	0.719	13	129	8	134	58	4 duplicate
13450	106 [733; Threitol (4TMS)]	28 Malic acid	62	0.653	0.876	7.703	0.654	14	128	17	125	12	30 duplicate
11777	106 [733; Threitol (4TMS)]	14 Fumaric acid	62	0.622	0.858	11.540	0.622	15	127	22	120	43	44 duplicate
14525	106 [733; Threitol (4TMS)]	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	62	0.620	0.871	6.388	0.678	16	126	20	122	2	23 duplicate
14627	106 [733; Threitol (4TMS)]	39 [829; 1-Phenylethanol (1TMS)]	61	0.616	0.877	8.732	0.667	17	125	16	126	23	24 duplicate
16770	106 [733; Threitol (4TMS)]	62 [812; D-Xylofuranose (4TMS)]	62	0.607	0.841	10.619	0.651	18	124	24	118	39	32 duplicate
12757	106 [733; Threitol (4TMS)]	22 [690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	51	0.589	0.813	12.827	0.601	19	123	31	111	52	60 duplicate
9341	106 [733; Threitol (4TMS)]	134 Isomaltose	62	0.579	0.880	17.796	0.695	20	122	15	127	83	13 original
16281	106 [733; Threitol (4TMS)]	56 [829; Orotic acid (3TMS)]	62	0.576	0.871	8.449	0.685	21	121	19	123	16	18 duplicate
11650	106 [733; Threitol (4TMS)]	13 Uridic	62	0.574	0.851	10.200	0.698	22	120	23	119	33	12 duplicate
19185	106 [733; Threitol (4TMS)]	104 [795; Erythritol (4TMS)]	61	0.573	0.810	6.698	0.632	23	119	32	110	5	40 duplicate
19031	106 [733; Threitol (4TMS)]	100 [857; Mannitol (6TMS)]	62	0.562	0.708	8.154	0.541	24	118	46	96	15	90 duplicate
9320	106 [733; Threitol (4TMS)]	113 Galactose-6-phosphate	61	0.552	0.829	8.962	0.642	25	117	27	115	25	36 original
12992	106 [733; Threitol (4TMS)]	24 [725; 2-Ketooctanoic acid (2TMS)]	62	0.552	0.865	26.472	0.691	26	114	21	121	122	15 duplicate

12397	106 [733; Threitol (4TMS)]	19	Alanine (BP) (3TMS)	62	0.552	0.800	7.559	0.602	27	115	35	107	10	59 duplicate
13223	106 [733; Threitol (4TMS)]	26	Citramalic acid	62	0.552	0.767	13.567	0.572	28	116	40	102	60	71 duplicate
15313	106 [733; Threitol (4TMS)]	46	Arabinose	62	0.551	0.875	9.729	0.703	29	113	18	124	28	10 duplicate
17366	106 [733; Threitol (4TMS)]	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	55	0.550	0.682	14.041	0.531	30	112	51	91	61	94 duplicate
13562	106 [733; Threitol (4TMS)]	29	Erythritol	62	0.547	0.814	8.679	0.655	31	111	30	112	20	29 duplicate
15683	106 [733; Threitol (4TMS)]	50	[746; Ribonic acid-1,4-lactone (3TMS)]	59	0.544	0.817	20.385	0.596	32	110	29	113	95	64 duplicate
12028	106 [733; Threitol (4TMS)]	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	62	0.543	0.838	12.765	0.713	33	109	25	117	51	5 duplicate
12638	106 [733; Threitol (4TMS)]	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	62	0.542	0.735	12.851	0.541	34	108	43	99	53	88 duplicate
18473	106 [733; Threitol (4TMS)]	88	Gluconic acid	62	0.540	0.774	7.179	0.666	35	107	38	104	6	25 duplicate
17001	106 [733; Threitol (4TMS)]	65	[646; 3-Deoxyglucitol (5TMS)]	61	0.540	0.885	9.125	0.690	36	106	12	130	26	17 duplicate
9332	106 [733; Threitol (4TMS)]	125	[692; Sucrose (6TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	62	0.527	0.807	25.526	0.599	37	105	34	108	119	61 original
9336	106 [733; Threitol (4TMS)]	129	[840; Maltose methoxymine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	57	0.521	0.836	7.660	0.658	38	104	26	116	11	27 original
11393	106 [733; Threitol (4TMS)]	11	Succinic acid	62	0.519	0.788	7.497	0.608	39	103	37	105	8	55 duplicate
19110	106 [733; Threitol (4TMS)]	102	[904; Galactose methoxymine (5TMS)]	62	0.511	0.637	10.217	0.542	40	102	58	84	34	87 duplicate
9321	106 [733; Threitol (4TMS)]	114	Fructose-6-phosphate	53	0.504	0.808	10.259	0.634	41	101	33	109	35	39 original
17640	106 [733; Threitol (4TMS)]	74	[912; Tetradecanoic acid (1TMS)]	62	0.502	0.718	8.808	0.548	42	100	45	97	24	84 duplicate
10733	106 [733; Threitol (4TMS)]	6	Glycerol	62	0.492	0.769	36.790	0.596	43	99	39	103	140	65 duplicate
12152	106 [733; Threitol (4TMS)]	17	[700; 2-methyl-1,2-propanediol (2TMS)]	62	0.491	0.798	12.311	0.560	44	98	38	106	46	68 duplicate
9339	106 [733; Threitol (4TMS)]	132	[895; Isomaltose methoxymine (8TMS)]	42	0.484	0.762	16.754	0.618	45	97	41	101	75	47 original
14828	106 [733; Threitol (4TMS)]	41	[639; Proline (2TMS)]	62	0.482	0.857	10.316	0.555	46	96	54	88	36	80 duplicate
9330	106 [733; Threitol (4TMS)]	123	[945; Galactofuranose-6-phosphate (7TMS)]	62	0.474	0.702	8.640	0.618	48	94	49	93	18	48 original
19148	106 [733; Threitol (4TMS)]	103	[848; Ethylamine (2TMS)]	61	0.472	0.638	10.575	0.611	49	93	57	85	38	54 duplicate
9327	106 [733; Threitol (4TMS)]	120	[945; Uridine (3TMS)]	53	0.462	0.292	9.939	0.615	50	92	74	68	31	50 original
12275	106 [733; Threitol (4TMS)]	18	[590; 1-Acetyl-2-thiohydantoin]	62	0.456	0.642	8.153	0.522	51	91	55	87	14	99 duplicate
11522	106 [733; Threitol (4TMS)]	12	Glycolic acid	61	0.455	0.733	13.551	0.563	52	90	44	98	59	76 duplicate
16365	106 [733; Threitol (4TMS)]	57	[757; 2-Desoxy-pentose-3-yose dimethoxymine (2TMS)]	53	0.451	0.827	8.100	0.544	53	89	28	114	13	33 duplicate
9319	106 [733; Threitol (4TMS)]	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	62	0.444	0.608	19.658	0.530	54	88	62	80	92	85 original
18420	106 [733; Threitol (4TMS)]	87	[945; beta-D-Glucopyranose (5TMS)]	60	0.434	0.744	28.808	0.529	55	87	42	100	128	96 duplicate
18675	106 [733; Threitol (4TMS)]	92	[680; Glycerol-2-phosphate (4TMS)]	52	0.415	0.704	8.702	0.553	56	86	48	94	21	82 duplicate
9342	106 [733; Threitol (4TMS)]	135	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	62	0.397	0.531	11.075	0.516	57	85	63	79	41	104 original
9334	106 [733; Threitol (4TMS)]	127	[777; Fructose-6-phosphate methoxymine (6TMS)]	39	0.387	0.506	8.720	0.617	58	84	64	78	22	49 original
9335	106 [733; Threitol (4TMS)]	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	44	0.385	0.615	6.598	0.588	59	83	61	81	3	67 original
18071	106 [733; Threitol (4TMS)]	101	[832; Dopamine (4TMS)]	62	0.384	0.506	10.076	0.555	60	82	65	77	32	79 duplicate
16037	106 [733; Threitol (4TMS)]	54	[NA]	53	0.379	0.704	13.383	0.571	61	81	47	95	57	72 duplicate
18311	106 [733; Threitol (4TMS)]	85	[528; Methylcitric acid (4TMS)]	46	0.372	0.677	8.666	0.540	62	80	52	90	19	91 duplicate
18021	106 [733; Threitol (4TMS)]	80	[772; D-Glucose (5TMS)]	60	0.336	0.664	24.884	0.489	63	79	53	89	117	115 duplicate
17960	106 [733; Threitol (4TMS)]	79	Glucose	62	0.332	0.685	29.313	0.620	64	78	50	92	131	45 duplicate
18626	106 [733; Threitol (4TMS)]	91	[766; beta-D-Methylglucopyranoside (4TMS)]	62	0.314	0.390	15.934	0.563	65	77	70	72	74	77 duplicate
19221	106 [733; Threitol (4TMS)]	105	[705; 2-Ketogluconic acid (5TMS)]	46	0.289	0.459	9.793	0.595	66	76	68	74	29	68 duplicate
18861	106 [733; Threitol (4TMS)]	96	myo-Inositol	47	0.271	0.221	21.913	0.369	67	75	79	63	106	140 duplicate
18905	106 [733; Threitol (4TMS)]	97	[756; beta-D-Methylglucopyranoside (4TMS)]	50	0.257	0.461	15.780	0.602	68	74	67	75	73	58 duplicate
18198	106 [733; Threitol (4TMS)]	83	Sorbitol	56	0.248	0.009	19.259	0.454	69	73	84	58	89	127 duplicate
9316	106 [733; Threitol (4TMS)]	109	Octadecanoic acid	62	0.226	0.616	17.031	0.608	70	72	60	82	79	56 original
9318	106 [733; Threitol (4TMS)]	111	[583; Erythritol (4TMS)]	42	0.222	0.310	24.217	0.429	71	71	73	69	113	132 original
9340	106 [733; Threitol (4TMS)]	133	[855; Squalene]	62	0.214	0.224	10.689	0.406	72	70	78	64	40	135 original
9347	106 [733; Threitol (4TMS)]	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	48	0.204	0.234	18.454	0.490	73	69	77	65	87	112 original
16925	106 [733; Threitol (4TMS)]	64	[789; Tyramine (3TMS)]	61	0.192	0.341	10.418	0.494	74	68	71	71	37	110 duplicate
11903	106 [733; Threitol (4TMS)]	15	Alanine	62	0.184	0.418	14.799	0.629	75	67	69	73	65	41 duplicate

18990	106 [733; Threitol (4TMS)]	99 [662; Ribose-5-phosphate methoxamine (BP) (5TMS)]	40	0.182	0.639	13.140	0.652	76	66	56	86	56	31 duplicate
18770	106 [733; Threitol (4TMS)]	94 Hexadecanoic acid	62	0.179	0.494	17.470	0.597	77	65	66	76	80	63 duplicate
9323	106 [733; Threitol (4TMS)]	116 [882; Pseudouridine (5TMS)]	30	0.172	0.331	11.484	0.520	78	64	72	70	42	100 original
9345	106 [733; Threitol (4TMS)]	138 [674; Ergosterol (1TMS)]	46	0.157	0.258	19.404	0.490	79	63	75	67	90	113 original
9348	106 [733; Threitol (4TMS)]	141 Larosta-8,24-dien-3-beta-ol	59	0.120	0.155	16.979	0.496	80	62	80	62	77	109 original
9325	106 [733; Threitol (4TMS)]	118 [928; Glucopyranose-6-phosphate (6TMS)]	57	0.071	0.240	12.721	0.399	81	61	76	68	49	138 original
9344	106 [733; Threitol (4TMS)]	137 Ergosterol	62	0.021	-0.024	14.847	0.493	82	60	86	56	68	111 original
17436	106 [733; Threitol (4TMS)]	71 [731; Erythrose (3TMS)]	62	0.009	0.044	11.708	0.550	83	59	83	59	45	83 duplicate
9343	106 [733; Threitol (4TMS)]	138 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.000	0.060	7.267	0.473	84	58	82	60	7	119 original
15407	106 [733; Threitol (4TMS)]	47 [NA]	62	-0.003	-0.027	14.556	0.534	85	57	87	55	64	92 duplicate
9337	106 [733; Threitol (4TMS)]	130 Trehalose	61	-0.011	-0.061	26.175	0.459	86	56	88	54	121	125 original
16448	106 [733; Threitol (4TMS)]	58 [636; 4R-Acetalamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	62	-0.029	-0.103	15.528	0.471	87	55	89	53	69	122 duplicate
9331	106 [733; Threitol (4TMS)]	124 [734; 1-Monooctadecyglycerol (2TMS); 1-Monohexadecenyglycerol (1TMS)]	57	-0.030	-0.150	26.579	0.459	88	54	91	51	123	124 original
18255	106 [733; Threitol (4TMS)]	84 Mannitol	60	-0.032	0.083	28.890	0.554	89	53	81	61	129	81 duplicate
9346	106 [733; Threitol (4TMS)]	139 [700; Ergosta-5,7-dien-3-ol]	37	-0.066	-0.218	21.328	0.437	90	52	98	44	104	130 original
9326	106 [733; Threitol (4TMS)]	119 [931; myo-Inositol-2-phosphate (7TMS)]	58	-0.079	-0.198	12.700	0.500	91	51	95	47	48	108 original
18723	106 [733; Threitol (4TMS)]	93 [607; Putrescine (4TMS)]	62	-0.088	0.000	20.034	0.458	92	50	85	57	94	126 duplicate
18576	106 [733; Threitol (4TMS)]	90 [910; D-Z-Hexadecanoic acid (1TMS)]	62	-0.091	-0.180	11.624	0.465	93	49	93	49	44	123 duplicate
14318	106 [733; Threitol (4TMS)]	75 [596; N-Acetylglutamic acid (2TMS)]	62	-0.108	-0.201	25.865	0.503	94	48	96	46	120	107 duplicate
17708	106 [733; Threitol (4TMS)]	35 Lysine	62	-0.111	-0.197	35.855	0.489	95	47	94	48	138	114 duplicate
15950	106 [733; Threitol (4TMS)]	53 Glycerol-2-phosphate	62	-0.123	-0.177	15.672	0.348	96	46	92	50	70	141 duplicate
10462	106 [733; Threitol (4TMS)]	4 Phosphoric acid	49	-0.138	-0.207	30.657	0.413	97	45	97	45	134	134 duplicate
9314	106 [733; Threitol (4TMS)]	107 9-(Z)-Octadecenoic acid	61	-0.146	-0.308	14.283	0.427	98	44	100	42	63	133 original
17505	106 [733; Threitol (4TMS)]	72 [919; D-Xylopyranose (4TMS)]	62	-0.164	-0.223	14.975	0.374	99	43	89	43	68	139 duplicate
17076	106 [733; Threitol (4TMS)]	66 Glycerc acid-3-phosphate	62	-0.236	-0.337	12.953	0.566	100	42	103	39	54	75 duplicate
10867	106 [733; Threitol (4TMS)]	7 Threonine	62	-0.245	-0.313	27.036	0.442	101	41	101	41	125	129 duplicate
10048	106 [733; Threitol (4TMS)]	1 [938; Sulfuric acid (2TMS)]	35	-0.264	-0.105	13.049	0.692	102	40	90	52	55	14 duplicate
16611	106 [733; Threitol (4TMS)]	60 Glycerol-3-phosphate	62	-0.292	-0.387	19.748	0.561	103	39	108	38	83	78 duplicate
17150	106 [733; Threitol (4TMS)]	67 Citric acid	62	-0.293	-0.403	21.228	0.541	104	38	107	35	101	89 duplicate
9315	106 [733; Threitol (4TMS)]	108 Octadecenoic acid	62	-0.289	-0.423	14.100	0.400	105	37	108	34	62	137 original
10187	106 [733; Threitol (4TMS)]	2 Serine	60	-0.324	-0.360	21.009	0.473	106	36	104	38	100	118 duplicate
13337	106 [733; Threitol (4TMS)]	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	51	-0.333	-0.720	24.382	0.548	107	35	122	20	115	85 duplicate
13763	106 [733; Threitol (4TMS)]	31 [622; Parabanic acid (2TMS)]	62	-0.369	-0.551	16.990	0.534	108	34	112	30	78	93 duplicate
15025	106 [733; Threitol (4TMS)]	43 [548; Leucine (2TMS)]	58	-0.379	-0.505	12.750	0.519	109	33	109	33	50	101 duplicate
11132	106 [733; Threitol (4TMS)]	9 Proline	61	-0.383	-0.382	27.676	0.472	110	32	105	37	127	121 duplicate
10325	106 [733; Threitol (4TMS)]	3 Ethanolamine	60	-0.417	-0.653	18.023	0.639	111	31	117	25	85	38 duplicate
14422	106 [733; Threitol (4TMS)]	37 Phenylalanine	62	-0.421	-0.534	20.708	0.507	112	30	111	31	97	105 duplicate
11000	106 [733; Threitol (4TMS)]	8 Isoleucine	53	-0.427	-0.324	20.442	0.401	113	29	102	40	96	136 duplicate
12875	106 [733; Threitol (4TMS)]	23 Homoserine	62	-0.443	-0.762	17.855	0.599	114	28	127	15	84	62 duplicate
15862	106 [733; Threitol (4TMS)]	52 [NA]	46	-0.443	-0.739	24.547	0.684	115	27	123	19	116	20 duplicate
16530	106 [733; Threitol (4TMS)]	59 Ornithine; Arginine	62	-0.448	-0.518	37.645	0.523	116	26	110	32	141	98 duplicate
18948	106 [733; Threitol (4TMS)]	98 [697; Ribose-5-phosphate methoxamine (5TMS)]	46	-0.451	-0.743	21.775	0.571	117	25	125	17	105	73 duplicate
13892	106 [733; Threitol (4TMS)]	32 [728; N,N-Dimethyllysine methyl ester]	61	-0.459	-0.663	23.451	0.811	118	24	118	24	110	53 duplicate
16948	106 [733; Threitol (4TMS)]	63 Glutamine	52	-0.483	-0.767	23.924	0.858	119	23	129	13	112	26 duplicate
16691	106 [733; Threitol (4TMS)]	61 [NA]	62	-0.510	-0.688	12.546	0.517	120	22	121	21	47	103 duplicate
14107	106 [733; Threitol (4TMS)]	34 Aspartic acid	62	-0.513	-0.584	30.710	0.480	121	21	113	29	135	117 duplicate
17223	106 [733; Threitol (4TMS)]	68 [570; Hypoxanthine (2TMS)]	20	-0.516	-0.900	15.773	0.605	122	20	139	3	72	57 duplicate
18081	106 [733; Threitol (4TMS)]	81 Tyrosine	62	-0.517	-0.686	32.947	0.703	123	19	120	22	137	9 duplicate

17835	106 [733; Threitol (4TMS)]	[826; beta-[[[5-methyl-2-phenylmethyl]amino- benzeneacetic acid methyl ester]	60 -0.519	-0.616	29.954	0.519	124	18	115	27	132	102 duplicate
15500	106 [733; Threitol (4TMS)]	48 Asparagine	62 -0.546	-0.826	19.638	0.644	125	17	134	8	91	34 duplicate
18816	106 [733; Threitol (4TMS)]	95 [770; 3,4,6-Trisubstitutedphenylmethanolamine (5TMS)]	48 -0.555	-0.770	21.268	0.567	126	16	130	12	102	74 duplicate
12518	106 [733; Threitol (4TMS)]	20 [619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	29 -0.587	-0.911	16.976	0.711	127	15	140	2	76	8 duplicate
11263	106 [733; Threitol (4TMS)]	10 Glycine	62 -0.571	-0.854	20.810	0.710	128	14	136	6	98	8 duplicate
15773	106 [733; Threitol (4TMS)]	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	43 -0.575	-0.766	21.298	0.545	129	13	128	14	103	86 duplicate
15218	106 [733; Threitol (4TMS)]	45 Homocysteine	59 -0.580	-0.742	25.125	0.504	130	12	124	18	118	108 duplicate
13673	106 [733; Threitol (4TMS)]	30 [815; Ethyl-3(2H)-thiophenone]	62 -0.583	-0.610	29.096	0.447	131	11	114	28	130	128 duplicate
14000	106 [733; Threitol (4TMS)]	33 Methionine	62 -0.589	-0.682	17.764	0.488	132	10	119	23	82	116 duplicate
9338	106 [733; Threitol (4TMS)]	131 [626; 5-Methylthioadenosine (3TMS)]	53 -0.591	-0.794	20.868	0.614	133	9	131	11	99	51 original
13108	106 [733; Threitol (4TMS)]	25 [709; 2,5-Diaminovalerolactam (2TMS)]	46 -0.596	-0.796	22.098	0.640	134	8	132	10	107	37 duplicate
14927	106 [733; Threitol (4TMS)]	69 Arginine	58 -0.600	-0.818	23.899	0.613	135	7	133	9	111	52 duplicate
15592	106 [733; Threitol (4TMS)]	42 Glutamic acid	58 -0.608	-0.853	30.846	0.472	136	6	116	26	136	120 duplicate
15592	106 [733; Threitol (4TMS)]	49 [877; Pyrophosphoric acid (4TMS)]	62 -0.633	-0.755	26.945	0.528	137	5	126	16	124	97 duplicate
18525	106 [733; Threitol (4TMS)]	89 [775; Dopamine (4TMS)]	35 -0.671	-0.883	22.196	0.625	138	4	138	4	108	43 duplicate
18140	106 [733; Threitol (4TMS)]	82 Lysine	37 -0.691	-0.962	22.763	0.721	139	3	141	1	109	3 duplicate
16123	106 [733; Threitol (4TMS)]	55 [612; 4-Aminobutyric acid (2TBS)]	41 -0.712	-0.834	24.329	0.619	140	2	135	7	114	46 duplicate
10598	106 [733; Threitol (4TMS)]	5 Leucine	43 -0.734	-0.876	17.749	0.578	141	1	137	5	81	69 duplicate
18577	107 9-(Z)-Octadecenoic acid	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	64 0.738	0.885	9.503	0.587	1	141	1	141	20	1 duplicate
12519	107 9-(Z)-Octadecenoic acid	20 [619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	31 0.578	0.591	20.771	0.445	2	140	8	134	106	19 duplicate
9360	107 9-(Z)-Octadecenoic acid	119 [931; myo-Inositol-2-phosphate (7TMS)]	64 0.563	0.789	10.228	0.475	3	139	2	140	28	8 original
9378	107 9-(Z)-Octadecenoic acid	137 Ergosterol	64 0.499	0.733	7.564	0.495	4	138	3	139	9	5 original
18771	107 9-(Z)-Octadecenoic acid	94 Hexadecenoic acid	64 0.485	0.355	10.246	0.585	5	137	26	116	27	2 duplicate
9349	107 9-(Z)-Octadecenoic acid	98 Octadecenoic acid	64 0.483	0.709	14.875	0.448	6	136	4	138	57	17 original
9350	107 9-(Z)-Octadecenoic acid	109 Octadecenoic acid	64 0.425	0.200	13.742	0.519	7	135	41	101	50	3 original
9392	107 9-(Z)-Octadecenoic acid	141 Lanosta-8,24-dien-3-beta-ol	61 0.424	0.677	22.682	0.497	8	134	5	137	116	4 original
9365	107 9-(Z)-Octadecenoic acid	124 [734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecenoylethylglycerol (1TMS)]	59 0.407	0.598	32.791	0.464	9	133	7	135	140	11 original
18141	107 9-(Z)-Octadecenoic acid	82 Lysine	39 0.341	0.501	10.972	0.474	10	132	13	129	32	9 duplicate
15863	107 9-(Z)-Octadecenoic acid	52 [NA]	46 0.333	0.579	25.912	0.384	11	131	9	133	124	73 duplicate
16849	107 9-(Z)-Octadecenoic acid	63 Glutamine	52 0.329	0.536	20.042	0.346	12	130	10	132	93	114 duplicate
9367	107 9-(Z)-Octadecenoic acid	128 [559; Erythritol (4TMS)]	45 0.295	0.357	13.073	0.403	13	129	24	118	44	48 original
17151	107 9-(Z)-Octadecenoic acid	67 Citric acid	64 0.284	0.339	10.604	0.447	14	128	27	115	30	18 duplicate
9352	107 9-(Z)-Octadecenoic acid	111 [583; Erythritol (4TMS)]	42 0.275	0.397	26.731	0.453	15	127	19	123	128	14 original
9368	107 9-(Z)-Octadecenoic acid	127 [777; Fructose-6-phosphate methoxamine (6TMS)]	39 0.268	0.275	9.434	0.396	16	126	37	105	19	59 original
9377	107 9-(Z)-Octadecenoic acid	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17 0.265	0.356	5.960	0.323	17	125	25	117	4	139 original
16124	107 9-(Z)-Octadecenoic acid	55 [612; 4-Aminobutyric acid (2TBS)]	43 0.262	0.622	28.923	0.426	18	124	6	136	137	30 duplicate
9373	107 9-(Z)-Octadecenoic acid	132 [895; Isomaltose methoxamine (8TMS)]	42 0.259	0.158	21.309	0.378	19	123	47	95	108	78 original
18256	107 9-(Z)-Octadecenoic acid	84 Mannitol	62 0.254	0.062	20.342	0.346	20	122	64	78	100	110 duplicate
16612	107 9-(Z)-Octadecenoic acid	60 Glycerol-3-phosphate	64 0.254	0.393	8.489	0.451	21	121	20	122	12	15 duplicate
18526	107 9-(Z)-Octadecenoic acid	89 [775; Dopamine (4TMS)]	35 0.247	0.535	20.452	0.338	22	120	11	131	101	127 duplicate
9369	107 9-(Z)-Octadecenoic acid	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45 0.244	0.067	9.262	0.402	23	119	63	79	18	51 original
14928	107 9-(Z)-Octadecenoic acid	42 Glutamic acid	60 0.241	0.311	19.564	0.378	24	118	30	112	88	80 duplicate
18817	107 9-(Z)-Octadecenoic acid	95 [770; 3,4,6-Trisubstitutedphenylmethanolamine (5TMS)]	50 0.233	0.361	27.498	0.366	25	117	22	120	131	94 duplicate
9372	107 9-(Z)-Octadecenoic acid	131 [626; 5-Methylthioadenosine (3TMS)]	55 0.228	0.358	24.567	0.418	26	116	23	119	119	36 original
18724	107 9-(Z)-Octadecenoic acid	93 [607; Putrescine (4TMS)]	60 0.214	0.074	25.302	0.376	27	115	62	80	122	84 duplicate
9381	107 9-(Z)-Octadecenoic acid	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49 0.211	0.469	24.661	0.420	28	114	15	127	120	34 original
17224	107 9-(Z)-Octadecenoic acid	68 [570; Hypoxanthine (2TMS)]	20 0.211	0.413	20.563	0.385	29	113	17	125	103	98 duplicate

14423	107 9-(Z)-Octadecenoic acid	37	Phenylalanine	64	0.209	0.327	9,650	0.361	30	112	28	114	21	101 duplicate
16593	107 9-(Z)-Octadecenoic acid	49	[877; Pyrophosphoric acid (4TMS)]	64	0.207	0.293	28,480	0.349	31	111	34	108	135	109 duplicate
8357	107 9-(Z)-Octadecenoic acid	116	[882; Pseudouridine (5TMS)]	30	0.205	0.526	13,112	0.381	32	110	12	130	45	76 original
17836	107 9-(Z)-Octadecenoic acid	77	benzeneacetic acid methyl ester	62	0.201	0.281	18,629	0.343	33	109	35	107	86	119 duplicate
10326	107 9-(Z)-Octadecenoic acid	3	Ethanolamine	62	0.200	0.405	19,136	0.410	34	108	18	124	87	42 duplicate
19222	107 9-(Z)-Octadecenoic acid	105	[705; 2-Ketogluconic acid (5TMS)]	48	0.200	0.188	11,740	0.407	35	107	43	89	38	44 duplicate
15774	107 9-(Z)-Octadecenoic acid	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	0.199	0.302	27,249	0.333	36	108	32	110	130	130 duplicate
16692	107 9-(Z)-Octadecenoic acid	61	[NA]	64	0.194	0.298	11,906	0.369	37	105	33	109	39	90 duplicate
15851	107 9-(Z)-Octadecenoic acid	53	Glycerol-2-phosphate	64	0.188	0.252	20,063	0.362	38	104	39	103	95	100 duplicate
9374	107 9-(Z)-Octadecenoic acid	133	[855; Squalene]	64	0.185	0.432	11,742	0.363	39	103	16	126	37	98 original
18082	107 9-(Z)-Octadecenoic acid	81	Tyrosine	64	0.176	0.364	21,453	0.400	40	102	21	121	109	54 duplicate
10599	107 9-(Z)-Octadecenoic acid	5	Leucine	45	0.172	0.163	15,989	0.347	41	101	48	86	85	113 duplicate
15123	107 9-(Z)-Octadecenoic acid	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	0.158	0.103	11,840	0.406	42	100	55	87	38	45 duplicate
17641	107 9-(Z)-Octadecenoic acid	74	[912; Tetradecanoic acid (1TMS)]	64	0.150	0.124	16,800	0.371	43	99	52	90	71	87 duplicate
18312	107 9-(Z)-Octadecenoic acid	85	[529; Methyicitric acid (4TMS)]	48	0.135	0.135	10,991	0.384	44	98	50	92	34	72 duplicate
9379	107 9-(Z)-Octadecenoic acid	138	[674; Ergosterol (1TMS)]	46	0.130	0.315	24,497	0.344	45	97	29	113	118	118 original
17296	107 9-(Z)-Octadecenoic acid	69	Arginine	60	0.123	0.190	12,179	0.403	46	96	42	100	41	49 duplicate
9380	107 9-(Z)-Octadecenoic acid	139	[700; Ergosta-5,7-dien-3-ol]	38	0.121	0.487	26,266	0.484	47	95	14	128	126	6 original
11264	107 9-(Z)-Octadecenoic acid	10	Glycine	64	0.115	0.281	8,530	0.409	48	94	36	106	13	43 duplicate
15501	107 9-(Z)-Octadecenoic acid	48	Asparagine	64	0.113	0.308	14,150	0.403	49	93	31	111	54	50 duplicate
9353	107 9-(Z)-Octadecenoic acid	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.110	0.054	26,227	0.377	50	92	65	77	125	81 original
9376	107 9-(Z)-Octadecenoic acid	122	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	0.102	0.094	4,450	0.352	51	91	58	84	1	106 original
9363	107 9-(Z)-Octadecenoic acid	120	[644; Erythritol (4TMS)]	52	0.097	0.092	22,633	0.378	52	90	59	83	115	79 original
13674	107 9-(Z)-Octadecenoic acid	30	[845; Ethyl-3-(H)-thiophenone]	64	0.087	0.128	16,164	0.341	53	89	51	91	81	121 duplicate
18991	107 9-(Z)-Octadecenoic acid	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	0.085	0.080	16,864	0.335	54	88	61	81	73	129 duplicate
16531	107 9-(Z)-Octadecenoic acid	59	Ornithine; Arginine	64	0.085	0.102	28,003	0.354	55	87	56	86	133	105 duplicate
11001	107 9-(Z)-Octadecenoic acid	8	Isoleucine	55	0.064	0.260	12,158	0.335	56	86	38	104	40	128 duplicate
19111	107 9-(Z)-Octadecenoic acid	102	[904; Galactose methoxyamine (5TMS)]	64	0.063	-0.015	15,136	0.332	57	85	73	69	61	133 duplicate
17437	107 9-(Z)-Octadecenoic acid	71	[731; Erythrose (3TMS)]	64	0.061	0.035	4,861	0.392	58	84	70	72	3	65 duplicate
14001	107 9-(Z)-Octadecenoic acid	33	Methionine	64	0.060	0.146	13,491	0.345	59	83	49	93	49	117 duplicate
16366	107 9-(Z)-Octadecenoic acid	57	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55	0.056	-0.097	15,309	0.432	60	82	83	59	62	26 duplicate
16038	107 9-(Z)-Octadecenoic acid	54	[NA]	55	0.051	-0.177	20,060	0.435	61	81	99	43	94	24 duplicate
18676	107 9-(Z)-Octadecenoic acid	92	[680; Glycerol-2-phosphate (4TMS)]	54	0.048	-0.399	14,900	0.397	62	80	129	13	58	58 duplicate
12758	107 9-(Z)-Octadecenoic acid	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.038	0.119	20,178	0.415	63	79	53	89	96	40 duplicate
14108	107 9-(Z)-Octadecenoic acid	34	Aspartic acid	64	0.033	0.042	20,294	0.331	64	78	69	73	97	135 duplicate
13893	107 9-(Z)-Octadecenoic acid	32	[729; N,N-Dimethyllysine methyl ester]	63	0.031	0.158	22,623	0.337	65	77	48	94	114	125 duplicate
11523	107 9-(Z)-Octadecenoic acid	12	Glycine acid	63	0.030	-0.104	20,527	0.349	66	76	86	56	102	108 duplicate
9371	107 9-(Z)-Octadecenoic acid	130	Trehalose	63	0.028	0.213	16,988	0.377	67	75	40	102	75	82 original
9361	107 9-(Z)-Octadecenoic acid	120	[945; Uridine (3TMS)]	54	0.019	-0.138	6,451	0.359	69	73	93	49	7	103 original
10049	107 9-(Z)-Octadecenoic acid	1	[938; Sulfuric acid (2TMS)]	36	0.013	-0.028	12,619	0.351	70	72	76	66	43	107 duplicate
10858	107 9-(Z)-Octadecenoic acid	7	Threonine	64	0.009	0.170	17,095	0.363	71	71	45	97	77	99 duplicate
9351	107 9-(Z)-Octadecenoic acid	110	[715; Erythritol (4TMS)]	54	0.008	-0.140	18,616	0.423	72	70	94	48	85	32 original
17506	107 9-(Z)-Octadecenoic acid	72	[919; D-Xylopyranose (4TMS)]	63	0.002	-0.022	16,807	0.400	73	69	74	68	72	56 duplicate
18906	107 9-(Z)-Octadecenoic acid	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	0.002	-0.140	16,525	0.425	74	68	95	47	69	31 duplicate
16949	107 9-(Z)-Octadecenoic acid	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	48	-0.005	0.175	25,586	0.298	75	67	44	98	127	141 duplicate
11778	107 9-(Z)-Octadecenoic acid	14	Fumaric acid	64	-0.007	-0.103	18,447	0.394	76	66	85	57	84	74 duplicate
19032	107 9-(Z)-Octadecenoic acid	100	[857; Mannitol (6TMS)]	64	-0.016	-0.090	8,579	0.338	77	65	80	62	15	124 duplicate
14319	107 9-(Z)-Octadecenoic acid	36	[596; N-Acetylglutamic acid (2TMS)]	64	-0.019	0.043	16,245	0.348	78	64	68	74	66	112 duplicate



13224	107 9-(Z)-Octadecenoic acid	26	Citramalic acid	64	-0.023	-0.053	4.658	0.404	79	63	77	65	2	47 duplicate
12276	107 9-(Z)-Octadecenoic acid	18	[590; 1-Acetyl-2-thiohydantoin]	64	-0.038	-0.096	9.872	0.355	80	62	82	60	22	104 duplicate
15219	107 9-(Z)-Octadecenoic acid	45	Homocysteine	61	-0.039	0.012	31.073	0.314	81	61	71	71	139	140 duplicate
13784	107 9-(Z)-Octadecenoic acid	31	[622; Parabanic acid (2TMS)]	64	-0.040	0.053	19.625	0.338	82	60	68	78	90	123 duplicate
13451	107 9-(Z)-Octadecenoic acid	28	Malic acid	64	-0.043	-0.122	7.978	0.384	83	59	90	52	11	71 duplicate
18189	107 9-(Z)-Octadecenoic acid	83	Sorbitol	58	-0.048	-0.070	11.142	0.331	84	58	78	64	35	134 duplicate
15684	107 9-(Z)-Octadecenoic acid	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	-0.049	-0.116	27.986	0.388	85	57	88	54	132	69 duplicate
11133	107 9-(Z)-Octadecenoic acid	9	Proline	63	-0.050	0.095	18.425	0.337	86	56	57	85	83	126 duplicate
9370	107 9-(Z)-Octadecenoic acid	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	-0.056	-0.167	16.901	0.427	87	55	98	44	74	27 original
12639	107 9-(Z)-Octadecenoic acid	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	-0.062	-0.098	6.197	0.370	88	54	84	58	6	89 duplicate
14729	107 9-(Z)-Octadecenoic acid	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.063	-0.120	21.454	0.393	89	53	89	53	110	63 duplicate
11394	107 9-(Z)-Octadecenoic acid	11	Succinic acid	64	-0.064	-0.240	9.978	0.368	90	52	108	34	23	91 duplicate
10463	107 9-(Z)-Octadecenoic acid	4	Phosphoric acid	51	-0.073	0.091	21.518	0.329	91	51	60	82	111	136 duplicate
12876	107 9-(Z)-Octadecenoic acid	23	Homoserine	64	-0.074	0.053	13.463	0.342	92	50	67	75	48	120 duplicate
9358	107 9-(Z)-Octadecenoic acid	117	[724; Glycerol (3TMS)]	56	-0.077	-0.136	15.311	0.373	93	49	92	50	63	85 original
9362	107 9-(Z)-Octadecenoic acid	121	[657; Erythritol (4TMS)]	55	-0.084	-0.178	22.499	0.405	94	48	100	42	113	46 original
18474	107 9-(Z)-Octadecenoic acid	88	Gluconic acid	64	-0.085	-0.191	12.230	0.393	95	47	101	41	42	82 duplicate
15026	107 9-(Z)-Octadecenoic acid	43	[548; Leucine (2TBS)]	60	-0.089	-0.143	10.989	0.363	96	46	96	46	33	97 duplicate
18387	107 9-(Z)-Octadecenoic acid	86	[793; D-Galactono-1,4-lactone (4TMS)]	61	-0.104	-0.386	20.628	0.464	97	45	127	15	104	101 duplicate
9356	107 9-(Z)-Octadecenoic acid	115	Glucose-6-phosphate	62	-0.104	-0.413	14.067	0.443	98	44	130	12	53	20 original
10188	107 9-(Z)-Octadecenoic acid	2	Serine	62	-0.107	0.115	13.768	0.327	99	43	54	88	51	138 duplicate
11651	107 9-(Z)-Octadecenoic acid	13	Uracil	64	-0.114	-0.224	10.404	0.400	100	42	105	37	29	35 duplicate
18771	107 9-(Z)-Octadecenoic acid	62	[812; D-Xylofuranose (4TMS)]	64	-0.117	-0.330	6.021	0.419	101	41	119	23	5	55 duplicate
17077	107 9-(Z)-Octadecenoic acid	66	Glyceric acid-3-phosphate	64	-0.125	-0.024	15.020	0.346	102	40	75	67	59	115 duplicate
15408	107 9-(Z)-Octadecenoic acid	47	[NA]	64	-0.129	-0.127	15.597	0.376	103	38	97	45	64	83 duplicate
13563	107 9-(Z)-Octadecenoic acid	29	Erythritol	64	-0.130	-0.222	13.306	0.390	104	39	104	38	46	67 duplicate
9375	107 9-(Z)-Octadecenoic acid	134	Isomaltose	64	-0.132	-0.305	17.805	0.420	105	37	116	28	80	33 original
14828	107 9-(Z)-Octadecenoic acid	39	[828; 1-Phenylethanol (1TMS)]	63	-0.137	-0.193	14.151	0.390	106	36	102	40	55	66 duplicate
15314	107 9-(Z)-Octadecenoic acid	46	Arabinose	63	-0.141	-0.359	17.312	0.448	107	35	125	17	78	16 duplicate
17002	107 9-(Z)-Octadecenoic acid	65	[646; 3-Deoxyglucitol (5TMS)]	63	-0.141	-0.287	21.098	0.440	108	34	113	29	107	22 duplicate
14526	107 9-(Z)-Octadecenoic acid	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.145	-0.234	10.806	0.402	109	33	107	35	31	53 duplicate
19257	107 9-(Z)-Octadecenoic acid	106	[733; Threitol (4TMS)]	62	-0.146	-0.308	14.283	0.427	110	32	117	25	56	28 duplicate
12398	107 9-(Z)-Octadecenoic acid	19	Alanine (BP) (3TMS)	64	-0.151	-0.303	9.192	0.477	111	31	115	27	17	7 duplicate
14829	107 9-(Z)-Octadecenoic acid	41	[639; Proline (2TMS)]	64	-0.152	-0.207	6.925	0.454	112	28	103	39	8	12 duplicate
12893	107 9-(Z)-Octadecenoic acid	24	[725; 2-Ketooctanoic acid (2TMS)]	64	-0.152	-0.284	20.333	0.417	113	29	112	30	99	39 duplicate
14214	107 9-(Z)-Octadecenoic acid	35	Pyroglutamic acid	64	-0.152	-0.462	28.738	0.417	114	30	133	9	138	38 duplicate
18862	107 9-(Z)-Octadecenoic acid	96	myo-Inositol	49	-0.153	-0.105	28.123	0.328	115	27	87	55	134	137 duplicate
17772	107 9-(Z)-Octadecenoic acid	76	Fructose	64	-0.156	-0.436	16.704	0.427	116	26	131	11	70	29 duplicate
16282	107 9-(Z)-Octadecenoic acid	56	[829; Orotic acid (3TMS)]	64	-0.157	-0.352	19.819	0.435	117	25	123	19	92	25 duplicate
18827	107 9-(Z)-Octadecenoic acid	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	-0.164	-0.230	19.802	0.345	118	24	106	36	91	116 duplicate
17707	107 9-(Z)-Octadecenoic acid	75	Lysine	64	-0.167	-0.002	26.821	0.340	119	23	72	70	129	122 duplicate
12029	107 9-(Z)-Octadecenoic acid	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	-0.174	-0.262	8.776	0.439	120	22	111	31	16	23 duplicate
9355	107 9-(Z)-Octadecenoic acid	114	Fructose-6-phosphate	53	-0.174	-0.332	17.080	0.385	121	21	121	21	76	70 original
9366	107 9-(Z)-Octadecenoic acid	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	-0.177	-0.532	21.559	0.380	122	20	138	4	112	77 original
17899	107 9-(Z)-Octadecenoic acid	78	Mannose	62	-0.177	-0.317	19.620	0.382	123	19	118	24	89	75 duplicate
19149	107 9-(Z)-Octadecenoic acid	103	[648; Ethylamine (2TMS)]	63	-0.178	-0.249	16.399	0.371	124	17	110	32	67	88 duplicate
19186	107 9-(Z)-Octadecenoic acid	104	[795; Erythritol (4TMS)]	63	-0.178	-0.295	13.811	0.396	125	18	114	28	52	60 duplicate
12153	107 9-(Z)-Octadecenoic acid	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	-0.181	-0.332	10.049	0.365	126	18	120	22	24	85 duplicate
13109	107 9-(Z)-Octadecenoic acid	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.191	-0.249	20.305	0.372	127	15	109	33	98	86 duplicate
9354	107 9-(Z)-Octadecenoic acid	113	Galactose-6-phosphate	62	-0.196	-0.492	17.743	0.414	128	14	136	6	79	41 original

18421	107 9-(Z)-Octadecenoic acid	87	[945; beta-D-Glucopyranose (5TMS)]	62	-0.214	-0.464	24.801	0.440	129	13	134	8	121	21 duplicate
9384	107 9-(Z)-Octadecenoic acid	123	[945; Galactofuranose-6-phosphate (7TMS)]	64	-0.234	-0.393	7.768	0.453	130	12	128	14	10	13 original
13338	107 9-(Z)-Octadecenoic acid	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	-0.235	-0.073	25.817	0.332	131	11	79	63	123	132 duplicate
16449	107 9-(Z)-Octadecenoic acid	58	[638; 4R-Acetaldo-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	-0.237	-0.095	8.551	0.333	132	10	81	61	14	131 duplicate
18072	107 9-(Z)-Octadecenoic acid	101	[832; Dopamine (4TMS)]	64	-0.239	-0.354	15.103	0.348	133	9	124	18	60	111 duplicate
17574	107 9-(Z)-Octadecenoic acid	73	[708; Glucose methoxyamine (5TMS)]	57	-0.242	-0.350	18.396	0.392	134	8	122	20	82	64 duplicate
17367	107 9-(Z)-Octadecenoic acid	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	-0.264	-0.490	10.128	0.395	135	7	135	7	25	61 duplicate
9359	107 9-(Z)-Octadecenoic acid	118	[928; Glucopyranose-6-phosphate (6TMS)]	58	-0.267	-0.442	16.449	0.387	136	6	132	10	68	68 original
10734	107 9-(Z)-Octadecenoic acid	8	Glycerol	64	-0.276	-0.542	29.144	0.418	137	5	139	3	138	37 duplicate
18022	107 9-(Z)-Octadecenoic acid	60	[772; D-Glucose (5TMS)]	62	-0.338	-0.502	20.750	0.368	138	4	137	5	105	93 duplicate
17961	107 9-(Z)-Octadecenoic acid	79	Glucose	64	-0.391	-0.555	23.308	0.389	139	3	140	2	117	57 duplicate
16926	107 9-(Z)-Octadecenoic acid	64	[788; Tyramine (3TMS)]	63	-0.396	-0.379	13.410	0.360	140	2	126	16	47	102 duplicate
11904	107 9-(Z)-Octadecenoic acid	15	Alanine	64	-0.422	-0.569	10.275	0.402	141	1	141	1	28	52 duplicate
18292	108 Octadecenoic acid	107	9-(Z)-Octadecenoic acid	64	-0.483	0.709	14.875	0.448	1	141	1	141	72	4 duplicate
9405	108 Octadecenoic acid	131	[626; 5-Methylthioadenosine (3TMS)]	55	0.426	0.417	12.078	0.383	2	140	25	117	44	65 original
12520	108 Octadecenoic acid	20	[618; 2,3,4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	0.424	0.496	12.987	0.428	3	139	12	130	57	16 duplicate
16125	108 Octadecenoic acid	55	[612; 4-Aminobutyric acid (2TBS)]	43	0.420	0.558	18.261	0.385	4	138	3	139	95	81 duplicate
9411	108 Octadecenoic acid	137	Ergosterol	64	0.405	0.645	13.685	0.388	5	137	2	140	62	75 original
17225	108 Octadecenoic acid	68	[570; Hypoxanthine (2TMS)]	20	0.400	0.485	12.841	0.288	6	136	16	126	54	140 duplicate
14929	108 Octadecenoic acid	42	Glutamic acid	60	0.395	0.491	29.770	0.396	7	135	14	128	123	56 duplicate
10327	108 Octadecenoic acid	3	Ethanolamine	62	0.373	0.543	6.963	0.436	8	134	4	138	8	10 duplicate
18578	108 Octadecenoic acid	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	64	0.368	0.504	6.888	0.394	9	133	10	132	7	64 duplicate
18142	108 Octadecenoic acid	82	Lysine	39	0.366	0.524	15.494	0.378	10	132	7	135	79	93 duplicate
9393	108 Octadecenoic acid	119	[931; myo-Inositol-2-phosphate (7TMS)]	64	0.360	0.494	7.507	0.398	11	131	13	129	14	67 original
18083	108 Octadecenoic acid	81	Tyrosine	64	0.357	0.540	34.658	0.442	12	130	5	137	134	6 duplicate
15775	108 Octadecenoic acid	51	[489; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	0.355	0.485	16.041	0.396	13	128	15	127	86	58 duplicate
10600	108 Octadecenoic acid	5	Leucine	45	0.339	0.377	8.170	0.392	14	128	32	110	18	69 duplicate
9398	108 Octadecenoic acid	124	[734; 1-Monodeoxyglycerol (2TMS); 1-Monohexadecanoglycerol (1TMS)]	59	0.335	0.513	19.078	0.362	15	127	8	134	99	116 original
16613	108 Octadecenoic acid	60	Glycerol-3-phosphate	64	0.332	0.506	22.260	0.390	16	126	9	133	111	72 duplicate
17837	108 Octadecenoic acid	77	[826; beta-[[[5-methyl-2-thienyl)methyl]eneamino-benzeneacetic acid methyl ester]	62	0.329	0.432	30.293	0.367	17	125	22	120	124	109 duplicate
11265	108 Octadecenoic acid	10	Glycine	64	0.328	0.496	19.305	0.414	18	124	11	131	100	26 duplicate
17152	108 Octadecenoic acid	67	Citric acid	64	0.324	0.411	24.889	0.411	19	123	26	116	118	33 duplicate
13894	108 Octadecenoic acid	32	[728; N,N-Dimethyllysine methyl ester]	63	0.315	0.467	12.467	0.392	20	122	19	123	47	87 duplicate
14424	108 Octadecenoic acid	37	Phenylalanine	64	0.310	0.456	23.750	0.365	21	121	20	122	113	112 duplicate
17297	108 Octadecenoic acid	69	Arginine	60	0.295	0.419	21.325	0.381	22	120	24	118	108	88 duplicate
18527	108 Octadecenoic acid	89	[775; Dopamine (4TMS)]	35	0.291	0.532	13.401	0.388	23	119	6	136	60	78 duplicate
9415	108 Octadecenoic acid	141	Lanosta-8,24-dien-3-beta-ol	61	0.287	0.479	9.820	0.425	24	118	17	125	28	17 original
16693	108 Octadecenoic acid	61	[NA]	64	0.283	0.285	6.001	0.384	25	117	46	96	5	82 duplicate
13875	108 Octadecenoic acid	30	[815; Ethyl-3(2H)-thiophenone]	64	0.275	0.326	30.711	0.375	26	116	38	104	125	98 duplicate
15864	108 Octadecenoic acid	52	[NA]	46	0.264	0.391	15.777	0.356	27	115	29	113	83	127 duplicate
16532	108 Octadecenoic acid	59	Ornithine; Arginine	64	0.261	0.321	42.173	0.374	28	114	40	102	139	101 duplicate
9383	108 Octadecenoic acid	109	Octadecanoic acid	64	0.249	0.079	23.772	0.409	29	113	63	79	114	35 original
18818	108 Octadecenoic acid	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	0.247	0.278	15.832	0.375	30	112	48	94	85	99 duplicate
14002	108 Octadecenoic acid	33	Methionine	64	0.245	0.339	10.169	0.369	31	111	35	107	33	105 duplicate
18772	108 Octadecenoic acid	94	Hexadecanoic acid	64	0.240	0.189	22.744	0.435	32	110	55	87	112	12 duplicate
15594	108 Octadecenoic acid	49	[877; Pyrophosphoric acid (4TMS)]	64	0.238	0.259	16.338	0.353	33	109	49	93	87	130 duplicate
9413	108 Octadecenoic acid	139	[700; Ergosta-5,7-dien-3-ol]	38	0.238	0.478	15.122	0.412	34	108	18	124	75	32 original



16927	108	Octadecanoic acid	64	[789; Tyramine (3TMS)]	63	-0.168	-0.169	5.738	0.367	85	57	74	68	4	108	duplicate
19187	108	Octadecenoic acid	104	[795; Erythritol (4TMS)]	63	-0.178	-0.172	9.252	0.437	86	56	75	67	26	9	duplicate
12640	108	Octadecenoic acid	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	-0.180	-0.249	18.078	0.364	87	55	83	59	93	115	duplicate
9397	108	Octadecenoic acid	123	[945; Galactofuranose-6-phosphate (7TMS)]	64	-0.188	-0.265	12.286	0.390	88	54	87	55	46	71	original
9399	108	Octadecenoic acid	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	-0.189	-0.480	34.310	0.393	89	53	123	19	133	66	original
11805	108	Octadecenoic acid	15	Alanine	64	-0.190	-0.298	20.303	0.382	90	52	89	53	105	87	duplicate
16367	108	Octadecenoic acid	57	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55	-0.191	-0.395	17.545	0.402	91	51	102	40	90	45	duplicate
13225	108	Octadecenoic acid	26	Citramalic acid	64	-0.196	-0.287	17.568	0.367	92	50	88	54	91	110	duplicate
12399	108	Octadecenoic acid	19	Alanine (BP) (3TMS)	64	-0.197	-0.258	13.882	0.395	93	48	88	56	64	60	duplicate
17962	108	Octadecenoic acid	79	Glucose	64	-0.197	-0.393	36.881	0.414	94	49	101	41	136	27	duplicate
12759	108	Octadecenoic acid	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	-0.198	-0.315	10.443	0.421	95	47	93	49	35	18	duplicate
18992	108	Octadecenoic acid	99	[682; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	-0.202	-0.328	9.945	0.368	96	46	96	46	29	106	duplicate
19033	108	Octadecenoic acid	100	[857; Mannitol (6TMS)]	64	-0.209	-0.336	10.378	0.377	97	45	98	44	34	95	duplicate
11524	108	Octadecenoic acid	12	Glyceric acid	63	-0.211	-0.422	9.161	0.405	98	44	109	33	23	40	duplicate
16039	108	Octadecenoic acid	54	[NA]	55	-0.213	-0.447	12.228	0.413	99	43	117	25	45	29	duplicate
19223	108	Octadecenoic acid	105	[705; 2-Ketogluconic acid (5TMS)]	48	-0.215	-0.418	15.365	0.431	100	42	106	36	78	14	duplicate
9396	108	Octadecenoic acid	122	[644; Erythritol (4TMS)]	52	-0.216	-0.320	14.240	0.420	101	41	94	48	67	21	original
9388	108	Octadecenoic acid	114	Fructose-6-phosphate	53	-0.218	-0.315	8.824	0.402	102	40	92	50	21	47	original
18677	108	Octadecenoic acid	92	[680; Glycerol-2-phosphate (4TMS)]	54	-0.223	-0.410	11.341	0.378	103	39	105	37	40	92	duplicate
14730	108	Octadecenoic acid	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.234	-0.312	35.965	0.405	104	38	90	52	135	39	duplicate
9395	108	Octadecenoic acid	121	[657; Erythritol (4TMS)]	55	-0.235	-0.312	12.054	0.412	105	37	91	51	43	31	original
9387	108	Octadecenoic acid	113	Galactose-6-phosphate	62	-0.241	-0.434	10.159	0.403	106	36	114	28	32	44	original
11779	108	Octadecenoic acid	14	Fumaric acid	64	-0.242	-0.397	7.659	0.395	107	35	103	39	15	59	duplicate
9384	108	Octadecenoic acid	110	[715; Erythritol (4TMS)]	54	-0.256	-0.419	13.621	0.452	108	34	107	35	61	2	original
13452	108	Octadecenoic acid	28	Malic acid	61	-0.262	-0.419	10.870	0.404	109	33	104	38	38	41	duplicate
15685	108	Octadecenoic acid	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	-0.264	-0.419	15.565	0.397	110	32	108	34	80	53	duplicate
11395	108	Octadecenoic acid	11	Succinic acid	64	-0.266	-0.438	9.601	0.387	111	31	115	27	79	79	duplicate
9391	108	Octadecenoic acid	117	[724; Glycerol (3TMS)]	56	-0.266	-0.352	10.757	0.440	112	30	99	43	37	7	original
17575	108	Octadecenoic acid	73	[708; Glucose methoxyamine (5TMS)]	57	-0.268	-0.370	11.892	0.388	113	29	100	42	42	74	duplicate
9403	108	Octadecenoic acid	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	-0.276	-0.431	14.885	0.405	114	28	113	29	73	38	original
14215	108	Octadecenoic acid	35	Pyroglutamic acid	64	-0.280	-0.505	43.095	0.414	115	27	131	11	140	28	duplicate
9389	108	Octadecenoic acid	115	Glucose-6-phosphate	62	-0.282	-0.465	26.916	0.397	116	26	120	22	118	54	original
16772	108	Octadecenoic acid	62	[812; D-Xylofuranose (4TMS)]	64	-0.285	-0.496	15.620	0.389	117	25	128	14	84	73	duplicate
18422	108	Octadecenoic acid	87	[945; beta-D-Glucopyranose (5TMS)]	62	-0.290	-0.449	37.461	0.384	118	24	118	24	137	114	duplicate
19258	108	Octadecenoic acid	106	[733; Threitol (4TMS)]	62	-0.299	-0.423	14.100	0.400	119	23	110	32	65	50	duplicate
17773	108	Octadecenoic acid	76	Fructose	64	-0.300	-0.493	28.228	0.419	120	22	125	17	120	23	duplicate
17900	108	Octadecenoic acid	78	Mannose	62	-0.300	-0.425	12.909	0.432	121	21	111	31	55	13	duplicate
18475	108	Octadecenoic acid	88	Gluconic acid	64	-0.301	-0.429	15.169	0.384	122	20	112	30	77	83	duplicate
14629	108	Octadecenoic acid	39	[829; 1-Phenylethanol (1TMS)]	63	-0.314	-0.468	19.786	0.414	123	19	121	21	101	25	duplicate
13594	108	Octadecenoic acid	29	Erythritol	64	-0.318	-0.496	7.056	0.394	124	18	129	13	9	63	duplicate
17003	108	Octadecenoic acid	65	[646; 3-Deoxyglucitol (5TMS)]	63	-0.319	-0.496	16.931	0.402	125	17	130	12	88	46	duplicate
18628	108	Octadecenoic acid	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	-0.319	-0.494	20.642	0.380	126	16	126	16	106	90	duplicate
15315	108	Octadecenoic acid	48	Arabinose	61	-0.320	-0.524	21.502	0.404	127	15	135	7	109	42	duplicate
18368	108	Octadecenoic acid	86	[793; D-Galactono-1,4-lactone (4TMS)]	61	-0.326	-0.554	25.347	0.435	128	14	138	4	117	11	duplicate
11652	108	Octadecenoic acid	13	Uracil	64	-0.327	-0.490	19.057	0.407	129	13	124	18	98	36	duplicate
9408	108	Octadecenoic acid	134	Isomaltose	64	-0.329	-0.518	28.325	0.410	130	12	133	9	121	34	original
18907	108	Octadecenoic acid	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	-0.332	-0.555	24.673	0.412	131	11	139	3	115	30	duplicate
10735	108	Octadecenoic acid	6	Glycerol	64	-0.336	-0.479	43.500	0.448	132	8	122	20	141	3	duplicate
14527	108	Octadecenoic acid	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.336	-0.495	10.111	0.380	133	9	127	15	31	89	duplicate

16283	108	Octadecanoic acid	56	[829; Orotic acid (3TMS)]	64	-0.336	-0.537	14,240	0.400	134	10	136	6	68	51 duplicate
17368	108	Octadecanoic acid	57	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	-0.342	-0.458	20,100	0.401	135	7	119	23	103	48 duplicate
12994	108	Octadecanoic acid	74	[725; 2-Ketotartaric acid (2TMS)]	64	-0.349	-0.519	34,250	0.404	136	8	134	8	132	43 duplicate
18023	108	Octadecanoic acid	80	[772; D-Glucose (5TMS)]	82	-0.353	-0.438	32,829	0.382	137	5	116	26	128	117 duplicate
12030	108	Octadecanoic acid	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	-0.359	-0.518	20,074	0.407	138	4	132	10	102	37 duplicate
12154	108	Octadecanoic acid	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	-0.364	-0.540	20,215	0.395	139	3	137	5	104	62 duplicate
19150	108	Octadecanoic acid	103	[648; Ethylamine (2TMS)]	63	-0.399	-0.559	18,144	0.395	140	2	140	2	94	61 duplicate
19073	108	Octadecanoic acid	101	[832; Dopamine (4TMS)]	64	-0.423	-0.608	14,466	0.399	141	1	141	1	70	52 duplicate
18773	109	Octadecanoic acid	94	Hexadecanoic acid	64	0.850	0.978	5,159	0.667	1	141	1	141	1	1 duplicate
9444	109	Octadecanoic acid	138	[874; Ergosterol (1TMS)]	46	0.697	0.818	31,639	0.496	2	140	5	137	126	39 original
9443	109	Octadecanoic acid	137	Ergosterol	64	0.691	0.611	13,042	0.562	3	139	18	124	10	8 original
9422	109	Octadecanoic acid	141	Lanosta-8,24-dien-3-beta-ol	61	0.675	0.674	29,209	0.570	4	138	11	131	119	7 original
18314	109	Octadecanoic acid	116	[882; Pseudouridine (5TMS)]	30	-0.674	0.681	21,482	0.487	5	137	10	132	69	58 original
9446	109	Octadecanoic acid	85	[528; Methylcitric acid (4TMS)]	48	0.624	0.849	19,913	0.486	6	136	4	138	59	47 duplicate
17643	109	Octadecanoic acid	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	49	0.614	0.617	32,289	0.480	7	135	16	126	128	50 original
9439	109	Octadecanoic acid	74	[912; Tetradecanoic acid (1TMS)]	64	0.588	0.901	19,585	0.553	8	134	2	140	53	12 duplicate
9432	109	Octadecanoic acid	133	[855; Squalene]	64	0.560	0.664	18,389	0.411	9	133	14	128	44	92 original
			126	[559; Erythritol (4TMS)]	45	0.545	0.876	19,641	0.603	10	132	3	139	55	5 original
			124	[734; 1-Monoleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]	59	0.455	0.410	39,761	0.423	11	131	43	99	140	82 original
9430	109	Octadecanoic acid	44	[910; 2-Ketogluconic acid methoxamine (4TMS)]	50	0.435	0.725	15,936	0.559	12	130	8	134	25	9 duplicate
15125	109	Octadecanoic acid	107	9-(2)-Octadecanoic acid	64	0.425	0.200	13,742	0.519	13	129	79	63	16	27 duplicate
17439	109	Octadecanoic acid	71	[731; Erythrose (3TMS)]	64	0.400	0.596	14,062	0.400	14	128	19	123	18	107 duplicate
9438	109	Octadecanoic acid	132	[895; Isomallose methoxamine (8TMS)]	42	0.396	0.470	27,594	0.390	15	127	39	103	112	112 original
9425	109	Octadecanoic acid	119	[931; myo-Inositol-2-phosphate (7TMS)]	64	0.387	0.364	18,961	0.458	16	126	50	92	47	65 original
18201	109	Octadecanoic acid	83	Sorbitol	58	0.383	0.386	12,275	0.354	17	125	47	95	4	127 duplicate
9417	109	Octadecanoic acid	111	[583; Erythritol (4TMS)]	42	0.382	0.501	35,568	0.410	18	124	33	109	135	93 original
9428	109	Octadecanoic acid	122	[644; Erythritol (4TMS)]	52	0.373	0.693	27,814	0.543	19	123	9	133	114	14 original
19113	109	Octadecanoic acid	102	[904; Galactose methoxamine (5TMS)]	64	0.365	0.531	22,663	0.401	20	122	31	111	81	104 duplicate
19034	109	Octadecanoic acid	100	[857; Mannitol (6TMS)]	64	0.339	0.535	16,443	0.425	21	121	29	113	30	79 duplicate
9416	109	Octadecanoic acid	110	[715; Erythritol (4TMS)]	54	0.336	0.670	22,500	0.606	22	120	12	130	79	3 original
			135												
9441	109	Octadecanoic acid		[902; Melibiose (8TMS); alpha-D-Gal-(1,8)-D-Glc (8TMS)]	64	0.330	0.585	14,231	0.386	23	119	23	119	20	113 original
9420	109	Octadecanoic acid	114	Fructose-6-phosphate	53	0.319	0.588	23,388	0.517	24	118	22	120	88	29 original
9418	109	Octadecanoic acid	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.317	0.528	33,350	0.398	25	117	32	110	131	108 original
9423	109	Octadecanoic acid	117	[724; Glycerol (3TMS)]	56	0.313	0.735	19,956	0.527	26	116	6	136	60	20 original
14731	109	Octadecanoic acid	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.309	0.664	19,805	0.540	27	115	13	129	58	15 duplicate
9427	109	Octadecanoic acid	121	[657; Erythritol (4TMS)]	55	0.302	0.732	26,067	0.524	28	114	7	135	116	24 original
9421	109	Octadecanoic acid	115	Glucose-6-phosphate	62	0.289	0.498	12,442	0.500	29	113	34	108	7	35 original
16614	109	Octadecanoic acid	60	Glycerol-3-phosphate	64	0.280	0.382	12,226	0.392	30	112	48	94	3	110 duplicate
9419	109	Octadecanoic acid	113	Galactose-6-phosphate	62	0.264	0.477	23,206	0.532	31	111	37	105	86	18 original
9445	109	Octadecanoic acid	139	[700; Ergosta-5,7-dien-3-ol]	38	0.263	0.200	34,600	0.410	32	110	80	62	133	94 original
12278	109	Octadecanoic acid	18	[590; 1-Acetyl-2-thiohydantoin]	64	0.262	0.591	17,401	0.476	33	109	20	122	36	52 duplicate
13453	109	Octadecanoic acid	28	Malic acid	64	0.255	0.559	15,956	0.468	34	108	26	116	27	57 duplicate
18579	109	Octadecanoic acid	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	64	0.252	0.057	19,691	0.502	35	107	95	47	56	34 duplicate
19326	109	Octadecanoic acid	108	Octadecenoic acid	64	0.249	0.079	23,772	0.409	36	106	93	49	90	96 duplicate
19188	109	Octadecanoic acid	104	[795; Erythritol (4TMS)]	63	0.244	0.590	19,367	0.484	37	105	21	121	50	49 duplicate
13226	109	Octadecanoic acid	26	Citramalic acid	64	0.239	0.558	12,397	0.413	38	104	27	115	6	90 duplicate
17774	109	Octadecanoic acid	76	Fructose	64	0.231	0.472	13,514	0.523	39	103	38	104	14	25 duplicate
17153	109	Octadecanoic acid	67	Citric acid	64	0.230	0.277	13,498	0.370	40	102	67	75	13	120 duplicate
12760	109	Octadecanoic acid	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.228	0.493	25,958	0.417	41	101	35	107	103	84 duplicate

19259	109	Octadecanoic acid	106	[733; Threitol (4TMS)]	62	0.226	0.616	17,031	0.608	43	99	17	125	32	2 duplicate
14216	109	Octadecanoic acid	35	Pyroglutamic acid	64	0.223	0.425	25,514	0.487	44	98	42	100	100	44 duplicate
11780	109	Octadecanoic acid	14	Fumaric acid	64	0.221	0.487	25,555	0.410	45	97	36	108	101	95 duplicate
12400	109	Octadecanoic acid	19	Alanine (BP) (3TMS)	64	0.208	0.571	13,987	0.497	46	96	25	117	17	38 duplicate
17901	109	Octadecanoic acid	78	Mannose	62	0.201	0.532	23,836	0.553	47	95	30	112	91	11 duplicate
14831	109	Octadecanoic acid	41	[639; Proline (2TMS)]	64	0.197	0.582	12,605	0.496	48	94	24	118	8	37 duplicate
12521	109	Octadecanoic acid	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	0.196	-0.547	25,994	0.598	49	93	134	8	104	6 duplicate
11525	109	Octadecanoic acid	12	Glyceric acid	63	0.189	0.379	27,640	0.403	50	92	49	93	113	102 duplicate
9429	109	Octadecanoic acid	123	[945; Galactofuranose-6-phosphate (7TMS)]	64	0.159	0.539	14,770	0.531	51	90	28	114	23	19 original
12641	109	Octadecanoic acid	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	0.159	0.440	12,119	0.418	52	91	40	102	2	83 duplicate
17576	109	Octadecanoic acid	73	[708; Glucose methoxamine (5TMS)]	57	0.157	0.622	22,464	0.525	53	89	15	127	78	23 duplicate
14425	109	Octadecanoic acid	37	Phenylalanine	64	0.152	0.161	13,386	0.320	54	88	83	59	11	138 duplicate
9426	109	Octadecanoic acid	120	[945; Uridine (3TMS)]	54	0.152	0.049	15,054	0.412	55	87	97	45	24	91 original
9433	109	Octadecanoic acid	127	[777; Fructose-6-phosphate methoxamine (8TMS)]	39	0.147	0.273	19,587	0.372	56	86	68	74	54	118 original
9434	109	Octadecanoic acid	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.137	0.217	17,949	0.397	57	85	77	65	39	109 original
14321	109	Octadecanoic acid	38	[596; N-Acetylglutamic acid (2TMS)]	64	0.124	0.265	15,948	0.364	58	84	69	73	26	123 duplicate
10328	109	Octadecanoic acid	3	Ethanolamine	62	0.113	-0.002	26,976	0.475	59	83	102	40	109	53 duplicate
16773	109	Octadecanoic acid	62	[812; D-Xylofuranose (4TMS)]	64	0.109	0.330	13,477	0.472	60	82	54	88	12	58 duplicate
18864	109	Octadecanoic acid	96	myo-Inositol	49	0.109	0.251	35,975	0.295	61	81	73	69	138	141 duplicate
9442	109	Octadecanoic acid	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.103	0.404	17,074	0.414	62	80	44	98	33	87 original
11396	109	Octadecanoic acid	11	Succinic acid	64	0.102	0.344	18,001	0.401	63	79	52	90	40	103 duplicate
18399	109	Octadecanoic acid	86	[793; D-Galactono-1,4-lactone (4TMS)]	61	0.101	0.394	19,209	0.535	64	78	46	98	48	16 duplicate
10870	109	Octadecanoic acid	7	Threonine	64	0.100	0.244	16,987	0.339	65	77	74	68	31	133 duplicate
9431	109	Octadecanoic acid	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	0.097	0.258	18,887	0.428	66	76	70	72	48	77 original
14528	109	Octadecanoic acid	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.091	0.432	18,004	0.486	67	75	41	101	41	48 duplicate
9436	109	Octadecanoic acid	130	Trehalose	63	0.086	0.085	17,295	0.327	68	74	90	52	35	137 original
18678	109	Octadecanoic acid	92	[680; Glycerol-2-phosphate (4TMS)]	54	0.082	0.135	22,090	0.428	69	73	86	56	76	78 duplicate
18094	109	Octadecanoic acid	81	Tyrosine	64	0.074	0.015	21,757	0.545	70	72	101	41	71	13 duplicate
17369	109	Octadecanoic acid	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	0.065	0.307	12,310	0.462	71	71	60	82	5	60 duplicate
18819	109	Octadecanoic acid	95	[770; 3,4,6-Trishydroxyphenylethanolamine (5TMS)]	50	0.063	-0.266	28,916	0.476	72	70	115	27	118	54 duplicate
15686	109	Octadecanoic acid	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	0.058	0.297	34,857	0.431	73	69	65	77	134	76 duplicate
18476	109	Octadecanoic acid	88	Gluconic acid	64	0.052	0.291	17,422	0.526	74	68	66	76	37	22 duplicate
17838	109	Octadecanoic acid	77	[826; beta-[[[5-methyl-2-thienyl)methyleneamino- benzeneacetic acid methyl ester]	62	0.039	-0.003	20,365	0.372	75	67	103	39	63	119 duplicate
16368	109	Octadecanoic acid	57	[757; 2-Desoxy-pentos-3-yose dimethoxamine (2TMS)]	55	0.038	0.300	19,572	0.432	76	66	63	79	52	75 duplicate
10736	109	Octadecanoic acid	6	Glycerol	64	0.038	0.231	26,453	0.448	77	65	75	67	107	71 duplicate
14630	109	Octadecanoic acid	39	[829; 1-Phenylethanol (1TMS)]	63	0.035	0.397	16,021	0.477	78	64	45	97	28	51 duplicate
14930	109	Octadecanoic acid	42	Glutamic acid	60	0.032	-0.084	22,506	0.314	79	63	105	37	80	140 duplicate
13565	109	Octadecanoic acid	29	Erythritol	64	0.030	0.304	21,342	0.459	80	62	62	80	67	64 duplicate
16040	109	Octadecanoic acid	54	[NA]	55	0.020	0.180	27,222	0.401	81	61	82	60	110	106 duplicate
9435	109	Octadecanoic acid	129	[840; Maltose methoxamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	0.006	0.315	21,940	0.475	82	60	57	85	75	55 original
17004	109	Octadecanoic acid	65	[846; 3-Deoxyglucitol (5TMS)]	63	0.006	0.358	24,857	0.487	83	59	51	91	98	45 duplicate
9440	109	Octadecanoic acid	134	Isomaltose	64	-0.001	0.334	16,163	0.509	84	58	53	89	29	32 original
11653	109	Octadecanoic acid	13	Uracil	64	-0.003	0.313	14,127	0.522	85	57	58	84	19	26 duplicate
15885	109	Octadecanoic acid	52	[NA]	46	-0.005	-0.301	30,495	0.495	86	56	118	24	123	40 duplicate
15316	109	Octadecanoic acid	46	Arabinose	64	-0.006	0.309	18,739	0.493	87	55	59	83	45	41 duplicate
16284	109	Octadecanoic acid	56	[829; Orotic acid (3TMS)]	64	-0.008	0.304	24,740	0.489	88	53	61	81	96	42 duplicate
17709	109	Octadecanoic acid	75	Lysine	64	-0.008	0.218	24,580	0.346	89	54	76	66	95	131 duplicate

12995	109	Octadecanoic acid	24	[725; 2-Ketooctanoic acid (2TMS)]	64	-0.009	0.323	18,129	0.526	90	52	58	86	42	21	129
19224	109	Octadecanoic acid	105	[705; 2-Ketogluconic acid (5TMS)]	48	-0.011	0.018	20,050	0.453	91	51	100	42	62	66	192
	109	Octadecanoic acid	58	[638; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]												
16451	109	Octadecanoic acid	79	Glucose	84	-0.015	0.189	14,386	0.351	92	50	81	61	21	129	164
17963	109	Octadecanoic acid	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	-0.016	0.253	20,647	0.452	93	49	72	70	65	67	179
12031	109	Octadecanoic acid	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	64	-0.023	0.299	12,649	0.556	94	48	64	78	9	10	120
15776	109	Octadecanoic acid	59	Ornithine; Arginine	44	-0.025	-0.363	32,957	0.444	95	47	121	121	129	72	157
16533	109	Octadecanoic acid	53	Glycerol-2-phosphate	64	-0.032	-0.030	26,418	0.345	96	46	104	38	106	132	165
15953	109	Octadecanoic acid	10	Glycine	64	-0.038	-0.361	28,648	0.384	97	45	120	22	117	114	159
11266	109	Octadecanoic acid	87	[945; beta-D-Glucopyranose (5TMS)]	64	-0.046	-0.364	17,615	0.488	98	44	122	20	38	43	112
184215	109	Octadecanoic acid	103	[648; Ethylamine (2TMS)]	63	-0.054	0.202	21,872	0.409	99	43	78	64	73	97	184
16928	109	Octadecanoic acid	64	[789; Tyramine (3TMS)]	63	-0.056	0.099	21,936	0.408	101	41	89	53	74	99	169
1212155	109	Octadecanoic acid	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	-0.062	0.255	13,686	0.436	102	40	71	71	15	74	121
9424	109	Octadecanoic acid	118	[928; Glucopyranose-6-phosphate (6TMS)]	58	-0.065	0.074	24,087	0.408	103	39	94	48	93	100	94
9437	109	Octadecanoic acid	131	[626; 5-Methylthioadenosine (3TMS)]	55	-0.068	-0.654	32,160	0.535	104	38	138	4	127	17	94
18256	109	Octadecanoic acid	84	Nannitol	62	-0.068	-0.381	23,450	0.375	105	37	124	18	89	116	182
16694	109	Octadecanoic acid	61	[NA]	64	-0.075	-0.256	21,630	0.414	106	36	112	30	70	88	166
17079	109	Octadecanoic acid	66	Glyceric acid-3-phosphate	64	-0.081	0.081	23,329	0.415	107	35	92	50	87	86	170
137676	109	Octadecanoic acid	30	[815; Ethyl-3(2H)-thiophenone]	64	-0.093	-0.163	20,529	0.359	108	34	109	33	64	124	137
11906	109	Octadecanoic acid	15	Alanine	64	-0.102	0.047	14,667	0.451	109	33	98	44	22	58	119
18993	109	Octadecanoic acid	99	[862; Ribose-5-phosphate methoxyamine (6P) (5TMS)]	41	-0.105	0.083	26,011	0.460	110	32	91	51	105	62	189
17226	109	Octadecanoic acid	68	[570; Hypoxanthine (2TMS)]	20	-0.105	-0.546	22,683	0.401	111	31	133	9	82	105	172
16126	109	Octadecanoic acid	55	[612; 4-Aminobutyric acid (2TBS)]	43	-0.107	-0.388	36,333	0.516	112	30	125	17	137	130	161
1373766	109	Octadecanoic acid	31	[622; Parabanic acid (2TMS)]	64	-0.111	-0.156	27,929	0.348	113	28	108	34	115	130	137
15503	109	Octadecanoic acid	48	Asparagine	64	-0.111	-0.394	24,790	0.459	114	29	126	16	97	63	155
17298	109	Octadecanoic acid	69	Arginine	60	-0.115	-0.375	19,996	0.463	115	27	123	19	81	59	172
18726	109	Octadecanoic acid	93	[607; Putrescine (4TMS)]	60	-0.121	-0.259	33,821	0.353	116	26	113	29	132	128	187
13895	109	Octadecanoic acid	32	[729; N,N-Dimethyllysine methyl ester]	63	-0.129	-0.148	30,824	0.460	117	25	108	36	124	61	138
11135	109	Octadecanoic acid	9	Proline	63	-0.131	0.139	19,381	0.332	118	24	85	57	51	135	111
10465	109	Octadecanoic acid	4	Phosphoric acid	51	-0.137	0.056	19,334	0.315	119	23	96	46	49	139	104
111003	109	Octadecanoic acid	8	Isoleucine	55	-0.145	0.123	17,247	0.331	120	22	87	55	34	136	111
18908	109	Octadecanoic acid	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	-0.145	-0.178	21,823	0.451	121	21	110	32	72	69	189
14003	109	Octadecanoic acid	33	Methionine	64	-0.145	-0.263	23,128	0.365	122	20	114	28	85	122	140
17508	109	Octadecanoic acid	72	[919; D-Xylopyranose (4TMS)]	63	-0.150	-0.294	25,900	0.378	123	19	117	25	102	115	175
18024	109	Octadecanoic acid	80	[772; D-Glucose (5TMS)]	62	-0.152	0.101	19,704	0.404	124	18	88	54	57	101	180
10190	109	Octadecanoic acid	2	Serine	62	-0.155	0.157	18,172	0.338	125	17	84	58	43	134	101
14110	109	Octadecanoic acid	34	Aspartic acid	64	-0.160	-0.244	21,377	0.368	126	16	111	31	68	121	141
19074	109	Octadecanoic acid	101	[632; Dopamine (4TMS)]	64	-0.174	-0.155	22,803	0.355	127	15	107	35	84	126	190
18629	109	Octadecanoic acid	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	-0.191	-0.277	27,397	0.374	128	14	116	26	111	117	186
18951	109	Octadecanoic acid	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	48	-0.209	-0.494	31,065	0.417	129	13	131	11	125	85	189
15595	109	Octadecanoic acid	49	[877; Pyrophosphoric acid (4TMS)]	64	-0.227	-0.660	38,535	0.504	130	12	139	3	139	33	155
16851	109	Octadecanoic acid	63	Glutamine	52	-0.252	-0.352	30,465	0.425	131	11	119	23	122	81	168
10601	108	Octadecanoic acid	5	Leucine	45	-0.259	-0.797	26,968	0.517	132	10	140	2	108	28	106
15221	109	Octadecanoic acid	45	Homocysteine	61	-0.259	-0.561	37,802	0.425	133	9	135	7	138	80	152
12878	109	Octadecanoic acid	23	Homoserine	64	-0.261	-0.470	23,954	0.413	134	8	129	13	92	89	128
18528	109	Octadecanoic acid	89	[775; Dopamine (4TMS)]	35	-0.284	-0.564	29,613	0.511	135	7	136	6	120	31	185
18143	109	Octadecanoic acid	82	Lysine	39	-0.314	-0.819	22,765	0.604	136	6	141	1	83	4	181
10051	109	Octadecanoic acid	1	[938; Sulfuric acid (2TMS)]	38	-0.321	-0.506	24,283	0.496	137	5	132	10	94	38	100
15028	109	Octadecanoic acid	43	[548; Leucine (2TBS)]	60	-0.323	-0.588	20,807	0.438	138	4	137	5	66	73	150
	109	Octadecanoic acid	47	[NA]	64	-0.339	-0.478	25,482	0.486	139	3	130	12	99	46	

13340	109	Octadecanoic acid	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	-0.348	-0.458	33.265	0.408	140	2	127	15	130	98 duplicate
13111	109	Octadecanoic acid	48	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.360	-0.470	30.293	0.449	141	1	128	14	121	70 duplicate
9454	110	[715; Erythritol (4TMS)]	117	[724; Glycerol (3TMS)]	52	0.916	0.948	5.412	0.670	1	141	4	138	4	18 original
19260	110	[715; Erythritol (4TMS)]	108	[733; Threitol (4TMS)]	52	0.902	0.980	9.825	0.731	2	140	1	141	25	1 duplicate
9459	110	[715; Erythritol (4TMS)]	122	[644; Erythritol (4TMS)]	49	0.900	0.974	7.325	0.716	3	139	3	139	8	3 original
9458	110	[715; Erythritol (4TMS)]	121	[657; Erythritol (4TMS)]	51	0.878	0.946	7.645	0.651	4	138	6	138	11	28 original
15128	110	[715; Erythritol (4TMS)]	44	[910; 2-Ketogluconic acid methoxamine (4TMS)]	49	0.871	0.978	5.171	0.684	5	137	2	140	3	20 duplicate
9463	110	[715; Erythritol (4TMS)]	128	[559; Erythritol (4TMS)]	45	0.792	0.948	3.192	0.729	6	136	5	137	1	2 original
17775	110	[715; Erythritol (4TMS)]	76	Fructose	54	0.779	0.926	27.214	0.655	7	135	7	135	120	22 duplicate
14732	110	[715; Erythritol (4TMS)]	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	54	0.712	0.876	35.791	0.639	8	134	9	133	135	37 duplicate
9452	110	[715; Erythritol (4TMS)]	115	Glucose-6-phosphate	53	0.701	0.892	26.973	0.648	9	133	8	134	119	29 original
14217	110	[715; Erythritol (4TMS)]	35	Pyroglutamic acid	54	0.651	0.866	42.455	0.614	10	132	11	131	140	49 duplicate
17902	110	[715; Erythritol (4TMS)]	78	Mannose	52	0.637	0.861	6.322	0.647	11	131	12	130	8	30 duplicate
17577	110	[715; Erythritol (4TMS)]	73	[708; Glucose methoxamine (5TMS)]	47	0.582	0.807	7.669	0.542	12	130	22	120	12	89 duplicate
13454	110	[715; Erythritol (4TMS)]	28	Malic acid	54	0.575	0.844	13.314	0.623	13	129	14	128	46	46 duplicate
19035	110	[715; Erythritol (4TMS)]	100	[657; Mannitol (6TMS)]	54	0.574	0.870	13.169	0.576	14	128	43	89	44	71 duplicate
11761	110	[715; Erythritol (4TMS)]	14	Fumaric acid	54	0.540	0.832	8.887	0.627	15	127	18	124	20	41 duplicate
17644	110	[715; Erythritol (4TMS)]	74	[912; Tetradecanoic acid (1TMS)]	54	0.537	0.744	8.321	0.545	16	126	34	108	17	88 duplicate
18370	110	[715; Erythritol (4TMS)]	86	[793; D-Galactono-1,4-lactone (4TMS)]	51	0.537	0.873	20.552	0.695	17	125	10	132	98	7 duplicate
13227	110	[715; Erythritol (4TMS)]	26	Citramelic acid	54	0.525	0.757	19.761	0.551	18	124	32	110	90	84 duplicate
14631	110	[715; Erythritol (4TMS)]	39	[829; 1-Phenylethanol (1TMS)]	54	0.523	0.843	16.398	0.655	19	123	15	127	67	23 duplicate
14529	110	[715; Erythritol (4TMS)]	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	54	0.522	0.833	11.368	0.643	20	122	17	125	32	33 duplicate
12761	110	[715; Erythritol (4TMS)]	22	[690; N,N-Di(2-Hydroxyethyl)-methanamine (2TMS)]	46	0.507	0.765	7.168	0.623	21	121	26	116	7	45 duplicate
19114	110	[715; Erythritol (4TMS)]	102	[904; Galactose methoxamine (5TMS)]	54	0.498	0.609	10.145	0.554	22	120	52	90	26	81 duplicate
9450	110	[715; Erythritol (4TMS)]	113	Galactose-6-phosphate	53	0.478	0.774	8.351	0.652	23	119	30	112	18	27 original
19189	110	[715; Erythritol (4TMS)]	104	[795; Erythritol (4TMS)]	53	0.451	0.665	10.406	0.606	25	117	45	97	28	57 duplicate
16774	110	[715; Erythritol (4TMS)]	62	[812; D-Xylofuranose (4TMS)]	54	0.451	0.781	17.864	0.845	26	116	27	115	78	32 duplicate
17370	110	[715; Erythritol (4TMS)]	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	47	0.449	0.539	21.503	0.521	27	115	60	82	102	95 duplicate
16285	110	[715; Erythritol (4TMS)]	56	[829; Orolic acid (3TMS)]	54	0.448	0.822	7.441	0.873	28	114	20	122	9	15 duplicate
12986	110	[715; Erythritol (4TMS)]	24	[725; 2-Ketooctanoic acid (2TMS)]	54	0.441	0.813	33.683	0.697	29	113	21	121	129	6 duplicate
9471	110	[715; Erythritol (4TMS)]	134	Isomaltose	54	0.438	0.835	26.210	0.702	30	111	16	126	117	5 original
9472	110	[715; Erythritol (4TMS)]	135		54	0.438	0.572	16.456	0.500	31	112	56	86	68	103 original
15687	110	[715; Erythritol (4TMS)]	50	[902; Malibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	53	0.437	0.771	13.100	0.615	32	110	31	111	43	47 duplicate
13566	110	[715; Erythritol (4TMS)]	29	Erythritol	54	0.433	0.742	10.392	0.636	33	109	35	107	27	38 duplicate
9451	110	[715; Erythritol (4TMS)]	114	Fructose-6-phosphate	45	0.432	0.775	7.599	0.683	34	108	29	113	10	9 original
17005	110	[715; Erythritol (4TMS)]	65	[646; 3-Deoxyglucitol (5TMS)]	54	0.431	0.844	7.803	0.682	35	107	13	129	13	10 duplicate
18477	110	[715; Erythritol (4TMS)]	88	Gluconic acid	54	0.430	0.707	13.986	0.682	36	106	41	101	54	11 duplicate
11654	110	[715; Erythritol (4TMS)]	13	Uracil	54	0.428	0.795	18.310	0.671	37	105	24	118	81	16 duplicate
18315	110	[715; Erythritol (4TMS)]	85	[529; Methylcitric acid (4TMS)]	38	0.428	0.741	10.688	0.593	38	104	36	106	29	68 duplicate
9449	110	[715; Erythritol (4TMS)]	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	53	0.428	0.597	13.777	0.515	39	103	55	87	52	98 original
12032	110	[715; Erythritol (4TMS)]	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	54	0.426	0.780	20.444	0.671	40	102	28	114	97	17 duplicate
11526	110	[715; Erythritol (4TMS)]	12	Glyceric acid	53	0.417	0.730	9.227	0.625	41	101	38	104	23	44 duplicate
15317	110	[715; Erythritol (4TMS)]	46	Arabinose	54	0.412	0.829	17.202	0.681	42	100	19	123	74	12 duplicate
9468	110	[715; Erythritol (4TMS)]	128	[940; Maltose methoxamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	53	0.408	0.787	9.054	0.660	43	99	25	117	22	21 original
12642	110	[715; Erythritol (4TMS)]	21	[676; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	54	0.407	0.614	19.957	0.593	44	98	50	92	91	66 duplicate
11397	110	[715; Erythritol (4TMS)]	11	Succinic acid	54	0.406	0.716	12.315	0.568	45	97	40	102	37	75 duplicate
9457	110	[715; Erythritol (4TMS)]	120	[945; Uridine (3TMS)]	48	0.394	0.216	15.112	0.612	46	96	76	68	58	52 original
12401	110	[715; Erythritol (4TMS)]	19	Alanine (BP) (3TMS)	54	0.391	0.722	15.100	0.612	47	95	39	103	57	51 duplicate
9469	110	[715; Erythritol (4TMS)]	132	[895; Isomaltose methoxamine (8TMS)]	39	0.387	0.746	9.821	0.628	48	94	33	109	24	40 original



9465	110 [715; Erythritol (4TMS)]	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	44	0.361	0.599	7.983	0.610	49	93	54	88	14	54 original
19152	110 [715; Erythritol (4TMS)]	103 [648; Ethylamine (2TMS)]	54	0.378	0.540	15.312	0.563	50	92	59	83	61	79 duplicate
9464	110 [715; Erythritol (4TMS)]	127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.374	0.534	5.832	0.605	51	91	62	80	5	59 original
9462	110 [715; Erythritol (4TMS)]	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	54	0.368	0.701	34.343	0.576	52	90	42	100	132	70 original
16369	110 [715; Erythritol (4TMS)]	57 [757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	51	0.360	0.789	11.421	0.680	53	89	23	119	33	13 duplicate
12156	110 [715; Erythritol (4TMS)]	17 [700; 2-methyl-1,2-propanediol (2TMS)]	54	0.358	0.733	20.357	0.600	54	88	37	105	98	62 duplicate
12279	110 [715; Erythritol (4TMS)]	18 [590; 1-Acetyl-2-thiohydantoin]	54	0.347	0.502	12.791	0.546	55	87	66	76	39	87 duplicate
19359	110 [715; Erythritol (4TMS)]	109 Octadecanoic acid	54	0.338	0.670	22.500	0.606	56	86	44	98	105	58 duplicate
19225	110 [715; Erythritol (4TMS)]	105 [705; 2-Ketogluconic acid (5TMS)]	48	0.337	0.508	11.583	0.642	57	85	65	77	34	35 duplicate
14832	110 [715; Erythritol (4TMS)]	41 [639; Proline (2TMS)]	54	0.336	0.609	17.038	0.558	58	84	51	91	72	80 duplicate
18774	110 [715; Erythritol (4TMS)]	94 Hexadecanoic acid	54	0.335	0.603	22.703	0.599	59	83	53	89	107	63 duplicate
18879	110 [715; Erythritol (4TMS)]	92 [680; Glyceral-2-phosphate (4TMS)]	49	0.330	0.546	8.500	0.598	60	82	57	85	19	64 duplicate
10737	110 [715; Erythritol (4TMS)]	6 Glyceral	54	0.311	0.618	43.043	0.587	61	81	49	93	141	67 duplicate
9478	110 [715; Erythritol (4TMS)]	141 Lanosta-8,24-dien-3-beta-ol	51	0.291	0.350	12.221	0.564	62	80	70	72	36	78 original
9460	110 [715; Erythritol (4TMS)]	123 [945; Galactofuranose-6-phosphate (7TMS)]	54	0.286	0.538	15.286	0.626	63	79	61	81	59	42 original
19075	110 [715; Erythritol (4TMS)]	101 [832; Dopamine (4TMS)]	54	0.283	0.387	13.891	0.494	64	78	68	74	53	105 duplicate
9477	110 [715; Erythritol (4TMS)]	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	39	0.282	0.323	13.704	0.523	65	77	72	70	51	92 original
9448	110 [715; Erythritol (4TMS)]	111 [583; Erythritol (4TMS)]	37	0.273	0.367	18.242	0.453	66	76	69	73	80	117 original
18202	110 [715; Erythritol (4TMS)]	83 Sorbitol	48	0.261	0.060	23.844	0.461	67	75	85	57	113	115 duplicate
9475	110 [715; Erythritol (4TMS)]	138 [874; Ergosterol (1TMS)]	38	0.255	0.342	14.320	0.478	68	74	71	71	55	108 original
9453	110 [715; Erythritol (4TMS)]	116 [892; Pseudouridine (5TMS)]	23	0.233	0.622	8.131	0.609	69	73	48	94	15	55 original
18424	110 [715; Erythritol (4TMS)]	87 [945; beta-D-Glucopyranose (5TMS)]	52	0.223	0.642	36.980	0.580	70	72	47	95	136	69 duplicate
16041	110 [715; Erythritol (4TMS)]	54 [NA]	49	0.206	0.545	8.227	0.625	71	71	58	84	16	43 duplicate
18909	110 [715; Erythritol (4TMS)]	97 [756; beta-D-Methylglucopyranoside (4TMS)]	49	0.192	0.293	21.732	0.640	72	70	73	69	104	38 duplicate
9470	110 [715; Erythritol (4TMS)]	133 [855; Squalene]	54	0.191	0.185	12.984	0.401	73	69	79	63	41	138 original
9456	110 [715; Erythritol (4TMS)]	119 [931; myo-Inositol-2-phosphate (7TMS)]	54	0.178	0.109	17.691	0.511	74	67	82	60	76	97 original
18865	110 [715; Erythritol (4TMS)]	96 myo-Inositol	39	0.155	0.160	18.493	0.259	76	66	80	62	69	141 duplicate
18630	110 [715; Erythritol (4TMS)]	91 [766; beta-D-Methylglucopyranoside (4TMS)]	54	0.136	0.216	19.693	0.502	77	65	77	65	88	102 duplicate
17440	110 [715; Erythritol (4TMS)]	71 [731; Erythrose (3TMS)]	54	0.126	0.186	16.532	0.531	78	64	78	64	70	91 duplicate
18025	110 [715; Erythritol (4TMS)]	80 [772; D-Glucose (5TMS)]	52	0.104	0.511	33.286	0.539	79	63	64	78	128	90 duplicate
9473	110 [715; Erythritol (4TMS)]	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.103	0.230	4.671	0.474	80	62	75	67	2	109 original
9461	110 [715; Erythritol (4TMS)]	124 [734; 1-Monodecylglycerol (2TMS); 1-Monohexadecylglycerol (1TMS)]	49	0.102	0.019	20.158	0.447	81	61	87	55	93	123 original
17964	110 [715; Erythritol (4TMS)]	79 Glucose	54	0.075	0.441	37.514	0.643	82	60	67	75	137	34 duplicate
18727	110 [715; Erythritol (4TMS)]	93 [607; Putrescine (4TMS)]	51	0.060	0.077	15.522	0.426	83	59	84	58	64	130 duplicate
9455	110 [715; Erythritol (4TMS)]	118 [928; Glucopyranose-6-phosphate (6TMS)]	52	0.057	0.267	11.298	0.446	84	58	74	68	31	124 original
18994	110 [715; Erythritol (4TMS)]	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	38	0.027	0.516	9.025	0.678	85	57	63	79	21	14 duplicate
19294	110 [715; Erythritol (4TMS)]	107 9-(Z)-Octadecenoic acid	54	0.008	-0.140	18.616	0.423	86	56	94	48	83	132 duplicate
18259	110 [715; Erythritol (4TMS)]	84 Mannitol	52	-0.006	0.058	34.171	0.600	87	55	86	56	131	60 duplicate
18580	110 [715; Erythritol (4TMS)]	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	54	-0.009	-0.038	13.327	0.433	88	54	90	52	47	127 duplicate
9476	110 [715; Erythritol (4TMS)]	139 [700; Ergosta-5,7-dien-3-ol]	31	-0.015	-0.051	16.819	0.404	89	53	91	51	71	137 original
15411	110 [715; Erythritol (4TMS)]	47 [NA]	54	-0.022	-0.005	15.309	0.614	90	52	88	54	60	48 duplicate
16929	110 [715; Erythritol (4TMS)]	64 [789; Tyramine (3TMS)]	53	-0.060	-0.030	11.604	0.449	91	51	89	53	35	122 duplicate
9467	110 [715; Erythritol (4TMS)]	130 Trehalose	53	-0.071	-0.108	31.292	0.507	92	50	93	49	123	99 original
17154	110 [715; Erythritol (4TMS)]	67 Citric acid	54	-0.082	-0.211	26.355	0.450	93	49	100	42	118	121 duplicate
14322	110 [715; Erythritol (4TMS)]	36 [596; N-Acetylglutamic acid (2TMS)]	54	-0.106	-0.183	30.914	0.568	94	48	99	43	122	76 duplicate
11907	110 [715; Erythritol (4TMS)]	15 Alanine	54	-0.113	0.120	22.886	0.647	95	47	81	61	108	31 duplicate
16452	110 [715; Erythritol (4TMS)]	58 [636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	54	-0.119	-0.141	20.717	0.497	96	45	95	47	100	104 duplicate

16615	110 [715; Erythritol (4TMS)]	60	Glycerol-3-phosphate	54	-0.119	-0.166	24.187	0.570	97	46	97	45	114	73 duplicate
17509	110 [715; Erythritol (4TMS)]	72	[919; D-Xylopyranose (4TMS)]	53	-0.141	-0.078	13.306	0.408	98	44	92	50	45	136 duplicate
17710	110 [715; Erythritol (4TMS)]	75	Lysine	54	-0.145	-0.176	40.491	0.523	99	44	98	44	138	83 duplicate
15954	110 [715; Erythritol (4TMS)]	53	Glycerol-2-phosphate	54	-0.164	-0.263	12.823	0.417	100	42	103	39	40	133 duplicate
10466	110 [715; Erythritol (4TMS)]	4	Phosphoric acid	41	-0.173	-0.161	33.707	0.432	101	41	96	46	130	128 duplicate
10871	110 [715; Erythritol (4TMS)]	7	Threonine	54	-0.177	-0.217	32.056	0.416	102	40	101	41	125	134 duplicate
15866	110 [715; Erythritol (4TMS)]	52	[NA]	36	-0.184	-0.592	20.189	0.652	103	39	120	22	94	28 duplicate
17080	110 [715; Erythritol (4TMS)]	66	Glyceric acid-3-phosphate	54	-0.216	-0.312	12.781	0.550	104	38	106	36	38	85 duplicate
19327	110 [715; Erythritol (4TMS)]	108	Octadecanoic acid	54	-0.256	-0.419	13.621	0.452	105	37	108	34	49	118 duplicate
10329	110 [715; Erythritol (4TMS)]	3	Ethanolamine	52	-0.275	-0.523	15.316	0.607	106	36	115	27	62	56 duplicate
14426	110 [715; Erythritol (4TMS)]	37	Phenylalanine	54	-0.286	-0.294	23.746	0.451	108	34	104	38	112	114 duplicate
10191	110 [715; Erythritol (4TMS)]	2	Serine	52	-0.302	-0.392	25.888	0.464	107	35	107	35	115	120 duplicate
11136	110 [715; Erythritol (4TMS)]	9	Proline	53	-0.306	-0.289	30.406	0.452	109	33	105	37	121	119 duplicate
13787	110 [715; Erythritol (4TMS)]	31	[622; Parabenic acid (2TMS)]	54	-0.307	-0.491	14.656	0.508	110	32	112	30	56	98 duplicate
18820	110 [715; Erythritol (4TMS)]	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	40	-0.351	-0.645	16.282	0.478	111	31	123	19	66	107 duplicate
16852	110 [715; Erythritol (4TMS)]	63	Glutamine	42	-0.357	-0.663	19.960	0.633	112	30	124	18	92	39 duplicate
	110 [715; Erythritol (4TMS)]		[826; beta-[(5-methyl-2-bienyl)methyl]enamine-											
17839	110 [715; Erythritol (4TMS)]	77	benzeneacetic acid methyl ester]	52	-0.371	-0.482	31.454	0.467	113	29	110	32	124	112 duplicate
16534	110 [715; Erythritol (4TMS)]	59	Ornithine; Arginine	54	-0.375	-0.434	41.501	0.466	114	28	109	33	139	113 duplicate
13341	110 [715; Erythritol (4TMS)]	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	43	-0.384	-0.705	22.505	0.522	115	27	126	16	106	94 duplicate
10052	110 [715; Erythritol (4TMS)]	1	[938; Sulfuric acid (2TMS)]	35	-0.385	-0.483	10.873	0.686	116	26	111	31	30	8 duplicate
10085	110 [715; Erythritol (4TMS)]	8	Tyrosine	54	-0.385	-0.552	34.607	0.703	117	25	117	25	133	4 duplicate
11004	110 [715; Erythritol (4TMS)]	81	Isoleucine	45	-0.388	-0.261	23.141	0.382	118	24	102	40	110	140 duplicate
16695	110 [715; Erythritol (4TMS)]	61	[NA]	54	-0.412	-0.495	13.635	0.455	119	23	113	28	50	116 duplicate
13896	110 [715; Erythritol (4TMS)]	32	[729; N,N-Dimethyllysine methyl ester]	53	-0.414	-0.593	21.433	0.613	120	22	121	21	101	50 duplicate
15504	110 [715; Erythritol (4TMS)]	48	Asparagine	54	-0.424	-0.773	18.643	0.600	121	21	132	10	84	61 duplicate
12879	110 [715; Erythritol (4TMS)]	23	Homoserine	54	-0.430	-0.741	19.094	0.569	122	20	129	13	85	74 duplicate
14111	110 [715; Erythritol (4TMS)]	34	Aspartic acid	54	-0.445	-0.512	34.759	0.428	123	19	114	28	134	128 duplicate
11267	110 [715; Erythritol (4TMS)]	10	Glycine	54	-0.455	-0.821	23.512	0.669	124	18	136	8	111	19 duplicate
15029	110 [715; Erythritol (4TMS)]	43	[548; Leucine (2TBS)]	50	-0.461	-0.568	15.791	0.425	125	17	119	23	65	131 duplicate
13677	110 [715; Erythritol (4TMS)]	30	[815; Ethyl-3(2H)-thiophenone]	54	-0.497	-0.530	32.484	0.409	126	16	116	26	127	135 duplicate
14004	110 [715; Erythritol (4TMS)]	33	Methionine	54	-0.509	-0.606	18.580	0.437	127	15	122	20	82	126 duplicate
14931	110 [715; Erythritol (4TMS)]	42	Glutamic acid	50	-0.510	-0.560	32.468	0.438	128	14	118	24	126	125 duplicate
15222	110 [715; Erythritol (4TMS)]	45	Homocysteine	51	-0.537	-0.693	19.599	0.467	129	13	125	17	87	111 duplicate
17289	110 [715; Erythritol (4TMS)]	69	Arginine	50	-0.541	-0.760	26.115	0.596	130	12	131	11	116	65 duplicate
18529	110 [715; Erythritol (4TMS)]	89	[775; Dopamine (4TMS)]	25	-0.547	-0.838	19.697	0.553	131	11	137	5	89	82 duplicate
13112	110 [715; Erythritol (4TMS)]	25	[709; 2,5-Diaminovalerolactam (2TMS)]	46	-0.552	-0.791	20.306	0.653	132	10	134	8	95	25 duplicate
18952	110 [715; Erythritol (4TMS)]	98	[697; Ribose-5-phosphate methoxamine (5TMS)]	40	-0.556	-0.783	18.225	0.548	133	9	133	9	79	86 duplicate
15777	110 [715; Erythritol (4TMS)]	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	34	-0.561	-0.732	17.597	0.480	134	8	128	14	75	108 duplicate
15598	110 [715; Erythritol (4TMS)]	49	[877; Pyrophosphoric acid (4TMS)]	54	-0.586	-0.717	22.931	0.503	135	7	127	15	109	101 duplicate
9468	110 [715; Erythritol (4TMS)]	131	[826; 5-Methylthiadenosine (3TMS)]	47	-0.593	-0.806	17.070	0.576	136	6	135	7	73	72 original
16127	110 [715; Erythritol (4TMS)]	65	[812; 4-Aminobutyric acid (2TBS)]	33	-0.610	-0.751	20.600	0.553	137	5	130	12	99	83 duplicate
17227	110 [715; Erythritol (4TMS)]	68	[570; Hypoxanthine (2TMS)]	13	-0.641	-0.913	13.426	0.383	138	4	140	2	48	139 duplicate
10602	110 [715; Erythritol (4TMS)]	5	Leucine	35	-0.677	-0.839	17.767	0.565	139	3	138	4	77	77 duplicate
	110 [715; Erythritol (4TMS)]													
12522	110 [715; Erythritol (4TMS)]	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	21	-0.686	-0.905	15.476	0.611	140	2	139	3	63	53 duplicate
18144	110 [715; Erythritol (4TMS)]	82	Lysine	29	-0.744	-0.948	21.528	0.654	141	1	141	1	103	24 duplicate
9483	111 [583; Erythritol (4TMS)]	116	[882; Pseudouridine (5TMS)]	23	0.542	0.660	12.523	0.382	1	140	3	138	28	71 original
18866	111 [583; Erythritol (4TMS)]	96	myo-Inositol	32	0.508	0.605	2.285	0.370	2	139	5	136	2	81 duplicate
19115	111 [583; Erythritol (4TMS)]	102	[904; Galactose methoxamine (5TMS)]	42	0.508	0.770	16.381	0.503	3	138	1	140	47	1 duplicate

9502	111 [583; Erythritol (4TMS)]	42	0.494	0.668	25.691	0.447	4	137	2	139	90	22 original
9505	111 [583; Erythritol (4TMS)]	32	0.435	0.549	5.643	0.469	5	136	9	132	7	13 original
9479	111 [583; Erythritol (4TMS)]	42	0.433	0.616	6.715	0.407	6	135	4	137	10	55 original
18775	111 [583; Erythritol (4TMS)]	42	0.394	0.555	34.424	0.428	7	134	8	133	114	39 duplicate
9499	111 [583; Erythritol (4TMS)]	34	0.387	0.535	12.599	0.340	8	133	29	112	30	101 original
9507	111 [583; Erythritol (4TMS)]	32	0.383	0.539	4.932	0.472	9	132	10	131	5	10 original
19360	111 [583; Erythritol (4TMS)]	42	0.382	0.501	35.568	0.410	10	131	14	127	118	53 duplicate
13455	111 [583; Erythritol (4TMS)]	28	0.370	0.497	23.358	0.394	11	130	16	125	80	62 duplicate
9504	111 [583; Erythritol (4TMS)]	42	0.361	0.442	25.375	0.398	12	129	23	118	85	69 original
18316	111 [583; Erythritol (4TMS)]	42	0.356	0.572	15.283	0.481	13	128	6	135	41	7 duplicate
9482	111 [583; Erythritol (4TMS)]	30	0.356	0.473	37.736	0.468	14	127	18	123	120	14 original
9496	111 [583; Erythritol (4TMS)]	42	0.340	0.366	19.605	0.439	15	126	38	103	65	28 original
19036	111 [583; Erythritol (4TMS)]	42	0.333	0.559	22.745	0.499	16	125	7	134	78	2 duplicate
11762	111 [583; Erythritol (4TMS)]	42	0.331	0.452	14.136	0.424	17	124	19	122	35	41 duplicate
9493	111 [583; Erythritol (4TMS)]	36	0.330	0.449	16.376	0.346	18	123	20	121	46	95 original
9480	111 [583; Erythritol (4TMS)]	42	0.324	0.443	16.980	0.421	19	122	22	119	49	45 original
17645	111 [583; Erythritol (4TMS)]	42	0.322	0.515	19.934	0.405	20	121	12	129	68	56 duplicate
18203	111 [583; Erythritol (4TMS)]	37	0.315	0.085	31.434	0.243	21	120	89	52	107	135 duplicate
16816	111 [583; Erythritol (4TMS)]	42	0.310	0.347	32.953	0.339	22	119	42	99	111	103 duplicate
9506	111 [583; Erythritol (4TMS)]	26	0.305	0.373	2.282	0.419	23	118	32	109	1	49 original
9500	111 [583; Erythritol (4TMS)]	41	0.303	0.507	19.309	0.397	24	117	13	128	62	61 original
9481	111 [583; Erythritol (4TMS)]	42	0.302	0.528	15.323	0.444	25	116	11	130	42	26 original
9508	111 [583; Erythritol (4TMS)]	39	0.301	0.437	9.575	0.447	26	115	24	117	17	23 original
13228	111 [583; Erythritol (4TMS)]	42	0.289	0.407	29.436	0.452	27	114	27	114	100	19 duplicate
15127	111 [583; Erythritol (4TMS)]	37	0.288	0.498	22.057	0.409	28	113	17	124	76	54 duplicate
17776	111 [583; Erythritol (4TMS)]	42	0.287	0.368	38.879	0.452	29	112	35	106	124	20 duplicate
14733	111 [583; Erythritol (4TMS)]	40	0.282	0.423	44.742	0.375	30	111	26	115	134	77 duplicate
9480	111 [583; Erythritol (4TMS)]	42	0.280	0.445	24.473	0.383	31	110	21	120	82	70 original
17441	111 [583; Erythritol (4TMS)]	42	0.278	0.348	25.437	0.374	32	109	41	100	86	80 duplicate
19295	111 [583; Erythritol (4TMS)]	42	0.275	0.397	26.731	0.453	33	108	28	113	92	18 duplicate
19391	111 [583; Erythritol (4TMS)]	37	0.273	0.367	18.242	0.453	34	107	36	105	55	16 duplicate
14427	111 [583; Erythritol (4TMS)]	42	0.268	0.325	34.148	0.321	35	106	45	96	113	111 duplicate
9503	111 [583; Erythritol (4TMS)]	17	0.265	0.256	11.211	0.316	36	105	67	74	19	113 original
14218	111 [583; Erythritol (4TMS)]	42	0.264	0.379	51.211	0.490	37	103	30	111	139	4 duplicate
12280	111 [583; Erythritol (4TMS)]	42	0.264	0.367	21.338	0.377	38	104	37	104	72	76 duplicate
9488	111 [583; Erythritol (4TMS)]	39	0.260	0.316	11.735	0.453	39	102	48	93	23	17 original
12762	111 [583; Erythritol (4TMS)]	22	0.260	0.322	11.537	0.438	40	101	46	95	20	30 duplicate
12643	111 [583; Erythritol (4TMS)]	42	0.247	0.368	29.866	0.389	41	100	34	107	101	65 duplicate
18581	111 [583; Erythritol (4TMS)]	90	0.245	0.376	19.300	0.425	42	97	31	110	61	40 duplicate
11527	111 [583; Erythritol (4TMS)]	42	0.245	0.368	12.399	0.401	43	98	33	108	27	58 duplicate
17155	111 [583; Erythritol (4TMS)]	67	0.245	0.264	35.255	0.374	44	99	65	76	115	79 duplicate
11398	111 [583; Erythritol (4TMS)]	42	0.231	0.424	21.661	0.423	45	96	25	116	73	43 duplicate
17803	111 [583; Erythritol (4TMS)]	40	0.228	0.352	18.220	0.483	46	95	40	101	54	8 duplicate
16930	111 [583; Erythritol (4TMS)]	64	0.222	0.499	17.150	0.392	47	93	15	126	50	64 duplicate
19261	111 [583; Erythritol (4TMS)]	106	0.222	0.310	24.217	0.429	48	94	53	88	81	38 duplicate
9489	111 [583; Erythritol (4TMS)]	122	0.215	0.286	13.462	0.435	49	92	56	85	33	32 original
10872	111 [583; Erythritol (4TMS)]	7	0.210	0.266	40.466	0.281	50	91	64	77	126	125 duplicate
9491	111 [583; Erythritol (4TMS)]	39	0.206	0.200	3.783	0.380	51	90	76	65	3	74 original
18821	111 [583; Erythritol (4TMS)]	28	0.201	0.098	6.131	0.277	52	89	86	55	8	129 duplicate

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136 [902; Melibiose (6TMS); alpha-D-Gal-(1,6)-D-Glc (6TMS)]  
 138 [674; Ergosterol (1TMS)]  
 112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]  
 94 Hexadecanoic acid  
 132 [895; Isomaltose methoxyamine (6TMS)]  
 140 [692; Ergosta-7,22-dien-3-ol (1TMS)]  
 109 Octadecanoic acid  
 28 Malic acid  
 137 Ergosterol  
 85 [529; Methylcitric acid (4TMS)]  
 115 Glucose-6-phosphate  
 119 [931; myo-Inositol-2-phosphate (7TMS)]  
 100 [857; Mannitol (6TMS)]  
 14 Fumaric acid  
 126 [559; Erythritol (4TMS)]  
 113 Galactose-6-phosphate  
 74 [912; Tetradecanoic acid (1TMS)]  
 83 Sorbitol  
 60 Glycerol-3-phosphate  
 139 [700; Ergosta-5,7-dien-3-ol]  
 133 [855; Squalene]  
 114 Fructose-6-phosphate  
 141 Lanosta-8,24-dien-3-beta-ol  
 26 Citramalic acid  
 44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]  
 76 Fructose  
 40 [680; 2,3-Dimethylsuccinic acid (2TMS)]  
 123 [945; Galactoturanose-6-phosphate (7TMS)]  
 71 [731; Erythrose (3TMS)]  
 107 9-(Z)-Octadecanoic acid  
 110 [715; Erythritol (4TMS)]  
 37 Phenylalanine  
 136 [748; D-Sedoheptulose-7-phosphate (7TMS)]  
 35 Pyroglutamic acid  
 121 [657; Erythritol (4TMS)]  
 22 [690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]  
 21 [678; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]  
 90 [910; 9-(Z)-Hexadecanoic acid (1TMS)]  
 12 Glycine acid  
 67 Citric acid  
 11 Succinic acid  
 78 Mannose  
 64 [789; Tyramine (3TMS)]  
 106 [733; Threitol (4TMS)]  
 122 [844; Erythritol (4TMS)]  
 7 Threonine  
 124 [734; 1-Monoleoylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]  
 95 [770; 3,4,6-Trisubstitutedphenylmethanolamine (5TMS)]

9484	111 [583; Erythritol (4TMS)]	117 [724; Glycerol (3TMS)]	38	0.195	0.225	18.832	0.475	53	88	73	68	58	8
12402	111 [583; Erythritol (4TMS)]	19 Alanine (BP) (3TMS)	42	0.192	0.312	25.904	0.472	54	87	50	81	91	11
17371	111 [583; Erythritol (4TMS)]	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	36	0.178	0.311	29.866	0.459	55	86	51	90	102	15
19180	111 [583; Erythritol (4TMS)]	104 [795; Erythritol (4TMS)]	41	0.168	0.204	19.921	0.343	58	85	75	66	67	98
17578	111 [583; Erythritol (4TMS)]	73 [708; Glucose methoxyamine (5TMS)]	37	0.159	0.321	18.065	0.346	57	84	47	94	51	96
14530	111 [583; Erythritol (4TMS)]	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	42	0.150	0.341	21.796	0.429	58	83	43	98	75	37
18478	111 [583; Erythritol (4TMS)]	88 Gluconic acid	42	0.145	0.276	25.466	0.375	59	82	62	79	88	78
11808	111 [583; Erythritol (4TMS)]	15 Alanine	42	0.141	0.241	31.040	0.344	60	81	71	70	106	98
16775	111 [583; Erythritol (4TMS)]	62 [812; D-Xylofuranose (4TMS)]	42	0.136	0.297	27.993	0.484	61	80	54	87	96	5
9492	111 [583; Erythritol (4TMS)]	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	42	0.134	0.243	43.857	0.435	62	79	70	71	132	33
16042	111 [583; Erythritol (4TMS)]	54 [NA]	40	0.131	0.356	14.684	0.418	63	78	39	102	39	51
10330	111 [583; Erythritol (4TMS)]	3 Ethanolamine	40	0.128	0.030	12.030	0.388	64	77	96	45	26	67
9494	111 [583; Erythritol (4TMS)]	127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	32	0.125	0.146	16.268	0.400	65	76	82	59	45	59
9495	111 [583; Erythritol (4TMS)]	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	35	0.119	0.253	20.637	0.381	66	75	69	72	70	73
19328	111 [583; Erythritol (4TMS)]	108 Octadecanoic acid	42	0.115	0.140	14.994	0.392	67	74	84	57	40	63
13587	111 [583; Erythritol (4TMS)]	29 Erythritol	42	0.113	0.314	18.190	0.422	68	73	49	92	53	44
14833	111 [583; Erythritol (4TMS)]	41 [639; Proline (2TMS)]	42	0.108	0.231	27.329	0.447	69	72	72	69	94	24
16880	111 [583; Erythritol (4TMS)]	92 [680; Glycerol-2-phosphate (4TMS)]	39	0.104	0.099	18.616	0.400	70	71	85	56	56	60
19153	111 [583; Erythritol (4TMS)]	103 [648; Ethylamine (2TMS)]	42	0.103	0.157	25.454	0.326	71	70	80	61	87	108
15318	111 [583; Erythritol (4TMS)]	46 Arabinose	42	0.089	0.282	30.228	0.444	72	69	59	82	104	25
18371	111 [583; Erythritol (4TMS)]	86 [793; D-Galactono-1,4-lactone (4TMS)]	40	0.085	0.291	33.823	0.473	73	68	55	88	112	9
18778	111 [583; Erythritol (4TMS)]	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	27	0.083	0.066	6.153	0.345	74	67	91	50	9	97
9501	111 [583; Erythritol (4TMS)]	134 Isomaltose	42	0.082	0.285	38.516	0.421	75	66	58	83	122	47
17840	111 [583; Erythritol (4TMS)]	[826; beta-[[[5-methyl-2-thienyl)methyl]amino- benzeneacetic acid methyl ester]	40	0.082	0.084	36.914	0.307	76	65	80	51	119	118
12033	111 [583; Erythritol (4TMS)]	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	42	0.080	0.281	31.563	0.434	77	64	60	81	108	34
12997	111 [583; Erythritol (4TMS)]	24 [725; 2-Ketooctanoic acid (2TMS)]	42	0.071	0.268	44.052	0.402	78	62	63	78	133	57
17965	111 [583; Erythritol (4TMS)]	79 Glucose	42	0.071	0.254	45.500	0.365	79	63	68	73	136	85
16286	111 [583; Erythritol (4TMS)]	56 [829; Orotic acid (3TMS)]	42	0.069	0.280	19.316	0.423	80	61	61	80	63	42
11655	111 [583; Erythritol (4TMS)]	13 Uracil	42	0.066	0.257	30.268	0.434	81	58	66	75	105	35
18631	111 [583; Erythritol (4TMS)]	91 [766; beta-D-Methylglucopyranoside (4TMS)]	42	0.066	0.058	25.530	0.329	82	59	94	47	89	105
18086	111 [583; Erythritol (4TMS)]	81 Tyrosine	42	0.066	0.004	41.363	0.332	83	60	101	40	130	104
9487	111 [583; Erythritol (4TMS)]	120 [945; Uridine (3TMS)]	38	0.054	-0.076	24.741	0.325	84	57	110	31	83	109
16696	111 [583; Erythritol (4TMS)]	61 [NA]	42	0.057	0.141	18.100	0.419	85	56	83	58	52	50
16370	111 [583; Erythritol (4TMS)]	57 [757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	38	0.041	0.330	25.196	0.435	86	55	44	97	84	31
17006	111 [583; Erythritol (4TMS)]	65 [846; 3-Deoxyglucitol (5TMS)]	41	0.039	0.310	21.274	0.450	87	53	52	89	71	21
14632	111 [583; Erythritol (4TMS)]	39 [829; 1-Phenylethanol (1TMS)]	41	0.039	0.288	29.976	0.417	88	54	57	84	103	52
15688	111 [583; Erythritol (4TMS)]	50 [746; Ribonic acid-1,4-lactone (3TMS)]	42	0.038	0.198	7.093	0.430	89	52	77	64	11	36
10182	111 [583; Erythritol (4TMS)]	2 Serine	41	0.029	0.094	27.771	0.259	90	51	67	54	95	132
17711	111 [583; Erythritol (4TMS)]	75 Lysine	42	0.029	0.094	48.048	0.280	91	50	88	53	137	127
19076	111 [583; Erythritol (4TMS)]	101 [832; Dopamine (4TMS)]	42	0.027	-0.003	22.395	0.281	92	49	102	39	77	126
14932	111 [583; Erythritol (4TMS)]	42 Glutamic acid	39	0.026	0.062	35.425	0.224	93	48	92	49	116	136
17228	111 [583; Erythritol (4TMS)]	68 [570; Hypoxanthine (2TMS)]	10	0.022	-0.094	4.191	0.018	94	47	114	27	4	140
9496	111 [583; Erythritol (4TMS)]	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	40	0.018	0.161	21.766	0.470	95	46	79	62	74	12
14323	111 [583; Erythritol (4TMS)]	36 [596; N-Acetylglutamic acid (2TMS)]	42	0.006	0.036	38.855	0.278	96	45	95	48	123	128
18260	111 [583; Erythritol (4TMS)]	84 Mannitol	40	0.003	-0.088	41.285	0.358	97	44	113	28	129	90
12157	111 [583; Erythritol (4TMS)]	17 [700; 2-methyl-1,2-propanediol (2TMS)]	42	0.001	0.217	31.730	0.389	98	43	74	67	110	66
11397	111 [583; Erythritol (4TMS)]	9 Proline	41	0.000	0.059	35.429	0.305	99	42	93	48	117	119
13897	111 [583; Erythritol (4TMS)]	32 [729; N,N-Dimethyllysine methyl ester]	41	-0.002	-0.033	14.520	0.303	100	41	107	34	38	120

15867	111 [583; Erythritol (4TMS)]	52 [NA]	28 -0.005	-0.114	9,054	0.257	101	40	116	25	16	133 duplicate
13878	111 [583; Erythritol (4TMS)]	30 [815; Ethyl-3(2H)-thiophenone]	42 -0.006	-0.047	38,317	0.282	102	39	108	33	121	124 duplicate
19226	111 [583; Erythritol (4TMS)]	105 [705; 2-Ketogluconic acid (5TMS)]	36 -0.008	-0.011	23,177	0.308	103	38	100	41	79	116 duplicate
14005	111 [583; Erythritol (4TMS)]	33 Methionine	42 -0.020	-0.078	19,712	0.351	104	37	112	29	66	94 duplicate
13788	111 [583; Erythritol (4TMS)]	31 [622; Parabanic acid (2TMS)]	42 -0.022	-0.076	12,586	0.363	105	36	111	30	29	86 duplicate
18995	111 [583; Erythritol (4TMS)]	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	32 -0.024	0.197	12,652	0.329	106	35	78	63	31	108 duplicate
10467	111 [583; Erythritol (4TMS)]	4 Phosphoric acid	33 -0.030	-0.024	40,682	0.264	107	34	105	36	127	130 duplicate
11005	111 [583; Erythritol (4TMS)]	8 Isoleucine	36 -0.032	0.157	28,846	0.231	108	33	81	60	83	137 duplicate
18728	111 [583; Erythritol (4TMS)]	93 [607; Putrescine (4TMS)]	39 -0.036	-0.019	10,231	0.290	109	32	104	37	18	121 duplicate
	111 [583; Erythritol (4TMS)]	[636; 4R-Acetamidino-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (6TMS)]										
16453	111 [583; Erythritol (4TMS)]	58 [1TMS]	42 -0.045	0.020	27,999	0.286	110	31	97	44	97	123 duplicate
18910	111 [583; Erythritol (4TMS)]	97 [756; beta-D-Methylglucopyranoside (4TMS)]	38 -0.050	-0.101	31,704	0.308	111	30	115	26	109	117 duplicate
17081	111 [583; Erythritol (4TMS)]	66 Glycolic acid-3-phosphate	42 -0.050	0.014	15,788	0.355	112	28	99	42	44	93 duplicate
10738	111 [583; Erythritol (4TMS)]	6 Glyceral	42 -0.050	-0.027	51,278	0.366	113	29	106	35	140	84 duplicate
9497	111 [583; Erythritol (4TMS)]	130 Trehalose	42 -0.052	0.018	40,203	0.324	114	27	98	43	125	110 original
16535	111 [583; Erythritol (4TMS)]	59 Ornithine; Arginine	42 -0.057	-0.053	48,684	0.260	115	26	109	32	138	131 duplicate
18425	111 [583; Erythritol (4TMS)]	87 [945; beta-D-Glucopyranose (5TMS)]	40 -0.062	-0.006	45,362	0.437	116	25	103	38	135	29 duplicate
17300	111 [583; Erythritol (4TMS)]	69 Arginine	39 -0.066	-0.198	29,152	0.341	117	24	122	19	99	100 duplicate
14112	111 [583; Erythritol (4TMS)]	3 Aspartic acid	42 -0.071	-0.125	41,735	0.257	118	23	117	24	131	134 duplicate
10603	111 [583; Erythritol (4TMS)]	5 Leucine	27 -0.083	-0.147	11,935	0.232	119	22	121	20	25	136 duplicate
11268	111 [583; Erythritol (4TMS)]	10 Glycine	42 -0.087	-0.206	28,850	0.420	120	21	124	17	98	48 duplicate
15223	111 [583; Erythritol (4TMS)]	45 Homocysteine	39 -0.093	-0.129	5,458	0.288	121	20	118	23	6	122 duplicate
9485	111 [583; Erythritol (4TMS)]	118 [928; Glucopyranose-6-phosphate (6TMS)]	40 -0.105	-0.282	16,505	0.382	122	19	129	12	48	72 original
12880	111 [583; Erythritol (4TMS)]	23 Homoserine	42 -0.102	-0.254	19,440	0.361	123	18	127	14	64	87 duplicate
18953	111 [583; Erythritol (4TMS)]	98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	27 -0.123	-0.200	7,316	0.314	124	17	123	18	13	114 duplicate
13342	111 [583; Erythritol (4TMS)]	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	34 -0.127	-0.231	13,119	0.204	125	16	126	15	32	139 duplicate
9498	111 [583; Erythritol (4TMS)]	131 [626; 5-Methylthiodenosine (3TMS)]	35 -0.167	-0.387	7,164	0.491	126	15	135	6	12	3 original
10053	111 [583; Erythritol (4TMS)]	1 [938; Sulfuric acid (2TMS)]	28 -0.163	-0.145	14,484	0.369	127	14	120	21	37	82 duplicate
16128	111 [583; Erythritol (4TMS)]	55 [612; 4-Aminobutyric acid (2TBS)]	26 -0.169	-0.305	7,935	0.311	128	13	131	10	14	115 duplicate
15505	111 [583; Erythritol (4TMS)]	48 Asparagine	42 -0.171	-0.298	18,823	0.358	129	11	119	22	128	75 duplicate
18026	111 [583; Erythritol (4TMS)]	80 [772; D-Glucose (5TMS)]	40 -0.177	-0.139	40,968	0.379	130	11	119	22	128	75 duplicate
17510	111 [583; Erythritol (4TMS)]	72 [919; D-Xylopyranose (4TMS)]	41 -0.178	-0.459	15,362	0.421	131	10	139	2	43	46 duplicate
15597	111 [583; Erythritol (4TMS)]	49 [877; Pyrophosphoric acid (4TMS)]	42 -0.182	-0.259	11,723	0.359	132	9	128	13	21	88 duplicate
18145	111 [583; Erythritol (4TMS)]	82 Lysine	23 -0.186	-0.317	19,116	0.357	133	8	132	9	59	91 duplicate
13113	111 [583; Erythritol (4TMS)]	25 [709; 2,5-Diaminovalerolactam (2TMS)]	36 -0.225	-0.226	14,187	0.366	134	7	125	16	36	83 duplicate
16853	111 [583; Erythritol (4TMS)]	83 Glutamine	38 -0.267	-0.321	14,077	0.356	135	6	134	7	34	92 duplicate
15412	111 [583; Erythritol (4TMS)]	47 [NA]	42 -0.301	-0.503	20,100	0.443	136	5	140	1	69	27 duplicate
15030	111 [583; Erythritol (4TMS)]	43 [548; Leucine (2TBS)]	39 -0.304	-0.318	19,165	0.329	137	4	133	8	60	107 duplicate
15955	111 [583; Erythritol (4TMS)]	53 Glycerol-2-phosphate	42 -0.350	-0.423	11,740	0.339	138	3	138	3	24	102 duplicate
	111 [583; Erythritol (4TMS)]											
12523		20 [619; 2,3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	16 -0.400	-0.394	8,074	0.386	139	2	137	4	15	68 duplicate
18530	111 [583; Erythritol (4TMS)]	89 [775; Dopamine (4TMS)]	23 -0.407	-0.388	11,723	0.318	140	1	136	5	22	112 duplicate
		135										
9531	112 [877; beta-D-Galactopyr	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	63 0.754	0.909	23,665	0.586	1	141	1	141	89	1 original
18116	112 [877; beta-D-Galactopyr	102 [904; Galactose methoxyamine (5TMS)]	63 0.732	0.854	11,928	0.576	2	140	2	140	36	2 duplicate
9512	112 [877; beta-D-Galactopyr	116 [882; Pseudouridine (5TMS)]	30 0.687	0.712	9,634	0.402	3	139	15	127	24	111 original
19037	112 [877; beta-D-Galactopyr	100 [857; Mannitol (6TMS)]	63 0.662	0.831	19,529	0.560	4	138	3	139	76	4 duplicate
9528	112 [877; beta-D-Galactopyr	132 [895; Isomaltose methoxyamine (8TMS)]	42 0.659	0.754	10,888	0.489	5	137	10	132	31	48 original
13456	112 [877; beta-D-Galactopyr	28 Malic acid	63 0.595	0.829	20,137	0.545	6	136	4	138	81	7 duplicate
11528	112 [877; beta-D-Galactopyr	12 Glyceric acid	62 0.570	0.793	6,839	0.497	7	135	6	136	10	45 duplicate
11399	112 [877; beta-D-Galactopyr	11 Succinic acid	63 0.556	0.775	18,141	0.503	8	134	8	134	72	40 duplicate

12763	112 [877; beta-D-Galactopyr	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.554	0.810	6.725	0.527	9	133	5	137	8	18 duplicate
9511	112 [877; beta-D-Galactopyr	115	Glucose-6-phosphate	62	0.542	0.622	36.705	0.522	10	132	36	106	119	21 original
11783	112 [877; beta-D-Galactopyr	14	Fumaric acid	63	0.538	0.761	8.836	0.504	11	131	7	135	21	39 duplicate
14734	112 [877; beta-D-Galactopyr	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	63	0.532	0.726	46.849	0.558	12	130	13	129	136	5 duplicate
14219	112 [877; beta-D-Galactopyr	35	Pyroglutamic acid	63	0.531	0.634	53.679	0.516	13	129	34	108	140	29 duplicate
16043	112 [877; beta-D-Galactopyr	54	[NA]	54	0.514	0.694	10.435	0.474	14	128	20	122	29	62 duplicate
12644	112 [877; beta-D-Galactopyr	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	63	0.506	0.714	28.293	0.476	15	128	14	128	101	58 duplicate
16776	112 [877; beta-D-Galactopyr	62	[812; D-Xylofuranose (4TMS)]	63	0.506	0.687	25.661	0.525	16	127	22	120	84	19 duplicate
13568	112 [877; beta-D-Galactopyr	29	Erythritol	63	0.493	0.743	13.875	0.543	17	125	11	131	51	10 duplicate
9522	112 [877; beta-D-Galactopyr	126	[559; Erythritol (4TMS)]	45	0.483	0.640	11.138	0.478	18	124	32	110	32	57 original
13229	112 [877; beta-D-Galactopyr	26	Citramalic acid	63	0.470	0.707	28.156	0.468	19	123	16	126	100	66 duplicate
17777	112 [877; beta-D-Galactopyr	76	Fructose	63	0.469	0.603	37.145	0.490	20	122	42	100	120	48 duplicate
14531	112 [877; beta-D-Galactopyr	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	63	0.467	0.770	17.892	0.521	21	121	9	133	70	23 duplicate
17646	112 [877; beta-D-Galactopyr	74	[912; Tetradecanoic acid (1TMS)]	63	0.461	0.704	15.189	0.501	22	120	17	125	58	41 duplicate
12998	112 [877; beta-D-Galactopyr	24	[725; 2-Ketocacetic acid (2TMS)]	63	0.460	0.698	44.280	0.518	23	119	19	123	131	26 duplicate
9524	112 [877; beta-D-Galactopyr	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.451	0.608	16.427	0.447	25	117	28	114	61	83 original
19262	112 [877; beta-D-Galactopyr	106	[733; Threitol (4TMS)]	62	0.444	0.608	19.658	0.530	26	116	41	101	78	14 duplicate
9518	112 [877; beta-D-Galactopyr	122	[644; Erythritol (4TMS)]	51	0.443	0.664	10.027	0.524	27	115	26	116	28	20 original
18867	112 [877; beta-D-Galactopyr	96	myo-Inositol	48	0.434	0.420	5.318	0.358	28	114	62	80	4	138 duplicate
18317	112 [877; beta-D-Galactopyr	85	[528; Methylcitric acid (4TMS)]	47	0.434	0.727	12.675	0.507	29	113	12	130	40	35 duplicate
12034	112 [877; beta-D-Galactopyr	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	83	0.434	0.701	29.506	0.544	30	112	18	124	106	9 duplicate
19422	112 [877; beta-D-Galactopyr	111	[583; Erythritol (4TMS)]	42	0.433	0.616	6.715	0.407	31	111	38	104	7	108 duplicate
9516	112 [877; beta-D-Galactopyr	88	Gluconic acid	54	0.433	0.191	22.233	0.528	32	110	80	62	85	15 original
18479	112 [877; beta-D-Galactopyr	120	[945; Uridine (3TMS)]	63	0.430	0.682	22.046	0.528	33	109	23	119	84	16 duplicate
19392	112 [877; beta-D-Galactopyr	110	[715; Erythritol (4TMS)]	53	0.428	0.587	13.777	0.515	34	108	49	93	49	31 duplicate
9521	112 [877; beta-D-Galactopyr	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	63	0.428	0.494	43.805	0.448	35	107	58	84	130	80 original
12281	112 [877; beta-D-Galactopyr	18	[590; 1-Acetyl-2-thiohydantoin]	63	0.427	0.632	18.038	0.435	36	106	35	107	71	89 duplicate
15319	112 [877; beta-D-Galactopyr	46	Arabinose	63	0.422	0.650	26.940	0.534	37	105	30	112	97	12 duplicate
9517	112 [877; beta-D-Galactopyr	31	[657; Erythritol (4TMS)]	54	0.421	0.580	7.182	0.476	38	104	50	92	11	59 original
14633	112 [877; beta-D-Galactopyr	39	[828; 1-Phenylethanol (1TMS)]	62	0.420	0.692	26.307	0.516	39	103	21	121	96	28 duplicate
17804	112 [877; beta-D-Galactopyr	78	Mannose	61	0.417	0.593	13.659	0.468	40	102	47	95	47	69 duplicate
15128	112 [877; beta-D-Galactopyr	44	[910; 2-Ketogluconic acid methoxymine (4TMS)]	49	0.413	0.598	17.415	0.414	41	101	44	98	66	101 duplicate
9530	112 [877; beta-D-Galactopyr	134	Isomaltose	63	0.409	0.676	36.360	0.514	42	100	24	118	118	33 original
16287	112 [877; beta-D-Galactopyr	58	[829; Orlic acid (3TMS)]	63	0.402	0.657	14.917	0.527	43	99	29	113	53	17 duplicate
9513	112 [877; beta-D-Galactopyr	117	[724; Glycerol (3TMS)]	56	0.397	0.610	13.876	0.492	44	98	40	102	50	47 original
12158	112 [877; beta-D-Galactopyr	17	[700; 2-methyl-1,2-propanediol (2TMS)]	63	0.394	0.641	26.168	0.475	45	97	31	111	104	61 duplicate
9523	112 [877; beta-D-Galactopyr	127	[777; Fructose-6-phosphate methoxymine (5TMS)]	39	0.393	0.594	11.704	0.481	46	96	46	96	35	55 original
18372	112 [877; beta-D-Galactopyr	86	[793; D-Galactono-1,4-lactone (4TMS)]	60	0.392	0.639	30.835	0.544	47	95	33	109	110	8 duplicate
9510	112 [877; beta-D-Galactopyr	114	Fructose-6-phosphate	53	0.389	0.596	10.003	0.483	48	94	45	97	27	51 original
9509	112 [877; beta-D-Galactopyr	113	Galactose-6-phosphate	62	0.389	0.542	12.478	0.481	49	93	53	89	37	72 original
17007	112 [877; beta-D-Galactopyr	65	[646; 3-Deoxyglucitol (5TMS)]	62	0.388	0.671	17.371	0.542	50	92	25	117	65	11 duplicate
18681	112 [877; beta-D-Galactopyr	92	[680; Glycerol-2-phosphate (4TMS)]	53	0.388	0.425	14.860	0.427	51	91	61	81	52	92 duplicate
9525	112 [877; beta-D-Galactopyr	129	[840; Maltose methoxymine (6TMS); alpha-D-Glc-(1,4)-D-Glc]	58	0.374	0.602	17.760	0.531	52	90	43	89	69	13 original
16371	112 [877; beta-D-Galactopyr													
15689	112 [877; beta-D-Galactopyr	50	[757; 2-Desoxy-pentose-3-yose dimethoxymine (2TMS)]	54	0.374	0.568	21.691	0.494	53	89	51	91	82	46 duplicate
11656	112 [877; beta-D-Galactopyr	70	[746; Ribonic acid-1,4-lactone (3TMS)]	60	0.355	0.615	5.104	0.500	54	88	39	103	3	42 duplicate
17372	112 [877; beta-D-Galactopyr	13	Uracil	63	0.353	0.662	27.475	0.546	55	87	27	115	98	6 duplicate
18996	112 [877; beta-D-Galactopyr	99	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	56	0.344	0.411	29.398	0.371	56	86	63	79	105	133 duplicate
19154	112 [877; beta-D-Galactopyr	103	[682; Ribose-5-phosphate methoxymine (8P) (5TMS)]	41	0.341	0.616	8.767	0.515	57	85	37	105	20	32 duplicate
			[648; Ethylamine (2TMS)]	62	0.339	0.524	22.563	0.521	58	84	55	87	86	22 duplicate

17579	112 [877; beta-D-Galactopyr 73	708; Glucose methoxyamine (5TMS)]	58	0.338	0.549	13.690	0.399	59	83	52	90	48	113 duplicate
19361	112 [877; beta-D-Galactopyr 109	Octadecanoic acid	63	0.317	0.528	33.350	0.398	60	82	54	88	114	114 duplicate
18776	112 [877; beta-D-Galactopyr 94	Hexadecanoic acid	63	0.300	0.523	33.254	0.455	61	81	56	86	113	74 duplicate
12403	112 [877; beta-D-Galactopyr 19	Alanine (BP) (3TMS)	63	0.292	0.510	22.757	0.498	62	80	57	85	87	44 duplicate
18261	112 [877; beta-D-Galactopyr 84	Mannitol	61	0.277	0.366	43.413	0.423	63	79	68	74	129	95 duplicate
18204	112 [877; beta-D-Galactopyr 83	Sorbitol	57	0.274	-0.088	32.164	0.370	64	78	91	51	111	134 duplicate
19077	112 [877; beta-D-Galactopyr 101	832; Dopamine (4TMS)]	63	0.261	0.383	19.281	0.442	65	77	64	78	74	85 duplicate
19227	112 [877; beta-D-Galactopyr 105	705; 2-Ketogluconic acid (5TMS)]	47	0.254	0.454	18.772	0.430	66	76	59	83	80	90 duplicate
9536	112 [877; beta-D-Galactopyr 140	692; Ergosta-7,22-dien-3-ol (1TMS)]	48	0.246	0.299	3.251	0.447	67	75	73	69	1	84 original
9519	112 [877; beta-D-Galactopyr 123	945; Galactofuranose-6-phosphate (7TMS)]	63	0.239	0.376	21.858	0.468	68	74	65	77	83	68 original
18632	112 [877; beta-D-Galactopyr 91	766; beta-D-Methylglucopyranoside (4TMS)]	63	0.238	0.369	24.165	0.440	69	73	67	75	80	86 duplicate
9537	112 [877; beta-D-Galactopyr 141	Lanosta-8,24-dien-3-beta-ol	60	0.228	0.346	6.811	0.422	70	72	69	73	9	96 original
14834	112 [877; beta-D-Galactopyr 41	639; Proline (2TMS)]	63	0.226	0.426	25.003	0.456	71	60	82	93	73 duplicate	
9534	112 [877; beta-D-Galactopyr 138	674; Ergosterol (1TMS)]	46	0.223	0.374	4.793	0.438	72	70	66	76	2	87 original
18911	112 [877; beta-D-Galactopyr 97	756; beta-D-Methylglucopyranoside (4TMS)]	51	0.208	0.310	30.211	0.417	73	69	72	70	108	100 duplicate
17442	112 [877; beta-D-Galactopyr 71	731; Erythrose (3TMS)]	63	0.189	0.177	23.597	0.455	74	68	81	61	88	75 duplicate
9533	112 [877; beta-D-Galactopyr 137	Ergosterol	63	0.177	0.177	24.870	0.360	75	67	82	60	91	137 original
8532	112 [877; beta-D-Galactopyr 136	748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.176	0.329	7.654	0.348	76	66	71	71	14	140 original
19191	112 [877; beta-D-Galactopyr 104	795; Erythritol (4TMS)]	62	0.176	0.266	15.976	0.447	77	65	75	67	60	82 duplicate
18426	112 [877; beta-D-Galactopyr 87	945; beta-D-Glucopyranose (5TMS)]	61	0.167	0.341	46.793	0.425	78	64	70	72	135	94 duplicate
16931	112 [877; beta-D-Galactopyr 64	789; Tyramine (3TMS)]	82	0.164	0.228	13.395	0.376	79	63	77	65	45	128 duplicate
9529	112 [877; beta-D-Galactopyr 133	855; Squalene	63	0.158	0.156	16.903	0.404	80	62	84	58	82	110 original
18582	112 [877; beta-D-Galactopyr 90	910; 9-(Z)-Hexadecanoic acid (1TMS)]	63	0.153	0.161	17.261	0.372	81	61	83	59	64	132 duplicate
10739	112 [877; beta-D-Galactopyr 8	Glycerol	63	0.143	0.283	54.175	0.393	82	60	74	68	141	120 duplicate
9515	112 [877; beta-D-Galactopyr 119	931; myo-Inositol-2-phosphate (7TMS)]	63	0.142	0.220	17.664	0.411	83	59	78	64	68	105 original
11909	112 [877; beta-D-Galactopyr 15	Alanine	63	0.126	0.139	30.021	0.482	84	58	86	56	107	53 duplicate
19286	112 [877; beta-D-Galactopyr 107	9-(Z)-Octadecenoic acid	63	0.110	0.054	26.227	0.377	85	57	88	54	95	128 duplicate
18729	112 [877; beta-D-Galactopyr 93	607; Putrescine (4TMS)]	59	0.109	0.105	8.256	0.379	86	58	87	55	16	128 duplicate
9535	112 [877; beta-D-Galactopyr 139	700; Ergosta-5,7-dien-3-ol	38	0.087	0.037	6.002	0.366	87	55	89	53	5	135 original
10054	112 [877; beta-D-Galactopyr 1	938; Sulfuric acid (2TMS)]	35	0.089	0.141	11.472	0.427	88	54	85	57	34	83 duplicate
17966	112 [877; beta-D-Galactopyr 79	Glucose	63	0.033	0.243	47.032	0.438	89	53	76	66	137	88 duplicate
18027	112 [877; beta-D-Galactopyr 80	772; D-Glucose (5TMS)]	61	0.025	0.201	42.051	0.373	90	52	79	63	128	131 duplicate
9520	112 [877; beta-D-Galactopyr 124	734; 1-Monooleoylglycerol (2TMS); 1-Monoheptadecanoylglycerol (1TMS)]	58	0.019	-0.127	8.688	0.406	91	51	95	47	19	109 original
15413	112 [877; beta-D-Galactopyr 47	[NA]	63	-0.028	-0.105	18.222	0.453	92	50	93	49	73	76 duplicate
16617	112 [877; beta-D-Galactopyr 60	Glycerol-3-phosphate	63	-0.053	-0.087	33.563	0.452	93	49	90	52	115	77 duplicate
17156	112 [877; beta-D-Galactopyr 67	Citric acid	63	-0.086	-0.125	36.033	0.413	94	48	94	48	117	102 duplicate
19329	112 [877; beta-D-Galactopyr 108	Octadecenoic acid	63	-0.089	-0.178	12.698	0.388	95	46	96	46	42	123 duplicate
15956	112 [877; beta-D-Galactopyr 53	Glycerol-2-phosphate	63	-0.089	-0.236	7.649	0.411	96	47	100	42	13	106 duplicate
14428	112 [877; beta-D-Galactopyr 37	Phenylalanine	63	-0.097	-0.192	34.952	0.422	97	45	97	45	116	98 duplicate
9514	112 [877; beta-D-Galactopyr 118	928; Glucopyranose-6-phosphate (6TMS)]	58	-0.099	-0.099	13.102	0.450	98	44	92	50	44	78 original
15868	112 [877; beta-D-Galactopyr 52	[NA]	46	-0.105	-0.335	12.558	0.513	99	43	105	37	38	34 duplicate
10873	112 [877; beta-D-Galactopyr 7	Threonine	63	-0.118	-0.202	42.514	0.374	100	42	99	43	128	130 duplicate
15779	112 [877; beta-D-Galactopyr 51	499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	63	-0.143	-0.439	9.105	0.483	101	41	118	24	22	52 duplicate
16129	112 [877; beta-D-Galactopyr 55	612; 4-Aminobutyric acid (2TBS)]	42	-0.143	-0.351	11.228	0.393	102	40	106	38	33	119 duplicate
16697	112 [877; beta-D-Galactopyr 61	[NA]	63	-0.148	-0.198	15.590	0.422	103	39	98	44	58	97 duplicate
17511	112 [877; beta-D-Galactopyr 72	919; D-Xylopyranose (4TMS)]	62	-0.149	-0.280	13.564	0.378	104	38	101	41	46	127 duplicate
18822	112 [877; beta-D-Galactopyr 95	770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	49	-0.190	-0.398	8.407	0.468	105	37	113	29	17	67 duplicate
10331	112 [877; beta-D-Galactopyr 3	Ethanolamine	61	-0.223	-0.382	10.802	0.449	106	36	111	31	30	79 duplicate
17229	112 [877; beta-D-Galactopyr 68	570; Hypoxanthine (2TMS)]	20	-0.242	-0.681	7.227	0.473	107	35	137	5	12	63 duplicate
9526	112 [877; beta-D-Galactopyr 130	Trehalose	62	-0.245	-0.369	42.056	0.412	108	34	109	33	127	104 original

10604	112 [877]: beta-D-Galactopyr	5	Leucine	44	-0.245	-0.530	12,951	0.519	109	33	129	13	43	25 duplicate
11006	112 [877]: beta-D-Galactopyr	8	Isoleucine	54	-0.259	-0.328	28,549	0.353	110	32	104	38	102	139 duplicate
14324	112 [877]: beta-D-Galactopyr	36	[596: N-Acetylglutamic acid (2TMS)]	63	-0.261	-0.367	40,848	0.412	111	30	108	34	123	103 duplicate
18087	112 [877]: beta-D-Galactopyr	81	Tyrosine	63	-0.261	-0.447	46,214	0.481	112	31	121	21	134	58 duplicate
16854	112 [877]: beta-D-Galactopyr	63	Glutamine	52	-0.267	-0.438	16,999	0.471	113	29	117	25	63	64 duplicate
14113	112 [877]: beta-D-Galactopyr	34	Aspartic acid	63	-0.268	-0.362	45,045	0.420	114	28	107	35	133	99 duplicate
17841	112 [877]: beta-D-Galactopyr	77	[826: beta-[[[5-methyl-2-thienyl)methyl]eneamino- benzenesuccinic acid methyl ester]	61	-0.274	-0.400	41,389	0.395	115	27	114	28	124	117 duplicate
13679	112 [877]: beta-D-Galactopyr	30	[815: Ethyl-3(2H)-thiophenone]	63	-0.276	-0.410	41,842	0.362	116	26	115	27	125	136 duplicate
12524	112 [877]: beta-D-Galactopyr	20	[619: 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	30	-0.278	-0.557	9,905	0.568	117	25	131	11	28	3 duplicate
10468	112 [877]: beta-D-Galactopyr	4	Phosphoric acid	50	-0.282	-0.294	44,289	0.337	118	24	102	40	132	141 duplicate
15506	112 [877]: beta-D-Galactopyr	48	Asparagine	63	-0.287	-0.509	19,659	0.488	119	23	128	14	79	50 duplicate
13898	112 [877]: beta-D-Galactopyr	32	[729: N,N-Dimethyllysine methyl ester]	62	-0.301	-0.496	15,933	0.520	120	22	127	15	59	24 duplicate
18531	112 [877]: beta-D-Galactopyr	89	[775: Dopamine (4TMS)]	35	-0.304	-0.594	15,266	0.448	121	21	133	9	57	81 duplicate
17082	112 [877]: beta-D-Galactopyr	66	Glycine acid-3-phosphate	63	-0.306	-0.379	12,673	0.506	122	20	110	32	39	38 duplicate
14006	112 [877]: beta-D-Galactopyr	33	Methionine	63	-0.308	-0.444	19,344	0.470	123	19	120	22	75	65 duplicate
17301	112 [877]: beta-D-Galactopyr	69	Arginine	59	-0.308	-0.597	32,365	0.518	124	18	134	8	112	27 duplicate
15224	112 [877]: beta-D-Galactopyr	45	Homocysteine	60	-0.308	-0.440	7,758	0.410	125	17	119	23	16	107 duplicate
17712	112 [877]: beta-D-Galactopyr	75	Lysine	63	-0.320	-0.389	52,051	0.397	126	16	112	30	138	115 duplicate
13789	112 [877]: beta-D-Galactopyr	31	[622: Perabanic acid (2TMS)]	63	-0.330	-0.533	9,838	0.462	127	15	130	12	25	70 duplicate
15598	112 [877]: beta-D-Galactopyr	49	[877: Pyrophosphoric acid (4TMS)]	63	-0.334	-0.476	12,692	0.383	128	14	125	17	41	125 duplicate
14933	112 [877]: beta-D-Galactopyr	42	Glutamic acid	59	-0.340	-0.490	40,659	0.395	129	13	126	16	122	116 duplicate
11269	112 [877]: beta-D-Galactopyr	10	Glycine	63	-0.350	-0.628	30,759	0.507	130	12	135	7	109	37 duplicate
16454	112 [877]: beta-D-Galactopyr	58	[636: 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	63	-0.354	-0.321	27,538	0.384	131	11	103	39	99	124 duplicate
9527	112 [877]: beta-D-Galactopyr	131	[626: 5-Methylthioadenosine (3TMS)]	54	-0.358	-0.580	6,637	0.461	132	10	132	10	6	71 original
11138	112 [877]: beta-D-Galactopyr	9	Proline	62	-0.363	-0.466	38,703	0.390	133	9	122	20	121	122 duplicate
18146	112 [877]: beta-D-Galactopyr	82	Lysine	38	-0.366	-0.642	24,873	0.515	134	8	136	6	92	30 duplicate
10193	112 [877]: beta-D-Galactopyr	2	Serine	61	-0.375	-0.426	29,016	0.401	135	7	116	26	103	112 duplicate
15031	112 [877]: beta-D-Galactopyr	43	[548: Leucine (2TBS)]	59	-0.377	-0.469	17,475	0.395	136	6	124	18	67	118 duplicate
18954	112 [877]: beta-D-Galactopyr	98	[697: Ribose-5-phosphate methoxyamine (5TMS)]	47	-0.380	-0.686	9,532	0.482	137	5	138	4	23	54 duplicate
12881	112 [877]: beta-D-Galactopyr	59	Ornithine; Arginine	63	-0.388	-0.467	53,359	0.391	138	4	123	19	139	121 duplicate
13343	112 [877]: beta-D-Galactopyr	27	[815: (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	63	-0.392	-0.708	19,583	0.507	139	3	140	2	77	36 duplicate
13114	112 [877]: beta-D-Galactopyr	25	[709: 2,5-Diaminvalerolactam (2TMS)]	52	-0.451	-0.704	15,138	0.498	140	2	139	3	55	43 duplicate
9538	113 Galactose-6-phosphate	114	Fructose-6-phosphate	47	-0.458	-0.718	15,067	0.475	141	1	141	1	54	60 duplicate
9539	113 Galactose-6-phosphate	115	Glucose-6-phosphate	53	0.890	0.978	2,175	0.685	1	141	1	141	1	1 original
9547	113 Galactose-6-phosphate	123	[945: Galactofuranose-6-phosphate (7TMS)]	62	0.739	0.987	25,551	0.571	2	140	2	140	119	34 original
14220	113 Galactose-6-phosphate	35	Pyroglutamic acid	62	0.722	0.854	11,603	0.643	3	139	8	134	46	8 original
17580	113 Galactose-6-phosphate	73	Glutamic acid	62	0.632	0.932	42,633	0.581	4	138	3	139	139	26 duplicate
12404	113 Galactose-6-phosphate	19	Alanine (BP) (3TMS)	55	0.605	0.815	5,609	0.537	5	137	13	129	4	52 duplicate
19192	113 Galactose-6-phosphate	104	[795: Erythritol (4TMS)]	62	0.599	0.830	11,978	0.568	6	136	9	133	49	39 duplicate
18205	113 Galactose-6-phosphate	83	Sorbitol	61	0.573	0.695	6,769	0.584	7	135	33	109	13	23 duplicate
17778	113 Galactose-6-phosphate	76	Fructose	56	0.569	0.102	23,013	0.404	8	134	78	64	111	121 duplicate
17805	113 Galactose-6-phosphate	78	Mannose	60	0.562	0.923	25,460	0.574	9	133	4	138	118	31 duplicate
19253	113 Galactose-6-phosphate	106	[733: Threitol (4TMS)]	62	0.559	0.824	5,685	0.519	10	132	11	131	5	64 duplicate
14735	113 Galactose-6-phosphate	40	[680: 2,3-Dimethylsuccinic acid (2TMS)]	61	0.552	0.829	8,962	0.642	11	131	10	132	29	9 duplicate
9545	113 Galactose-6-phosphate	121	[657: Erythritol (4TMS)]	62	0.538	0.745	36,283	0.535	12	130	21	121	136	55 duplicate
13457	113 Galactose-6-phosphate	28	Malic acid	53	0.528	0.743	9,170	0.563	13	129	22	120	32	44 original
9540	113 Galactose-6-phosphate	116	[882: Pseudouridine (5TMS)]	60	0.523	0.715	10,701	0.475	14	128	29	113	40	81 duplicate
				32	0.517	0.179	9,030	0.446	15	127	76	66	31	91 original



18318	113	Galactose-6-phosphate	85	[528; Methylcitric acid (4TMS)]	46	0.486	0.529	7.171	0.517	16	126	60	82	15	85 duplicate
17373	113	Galactose-6-phosphate	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	55	0.492	0.725	18.305	0.523	17	125	28	118	97	60 duplicate
9541	113	Galactose-6-phosphate	117	[724; Glycerol (3TMS)]	56	0.492	0.693	8.053	0.555	18	124	34	108	8	46 original
17867	113	Galactose-6-phosphate	79	Glucose	62	0.489	0.868	35.743	0.614	19	123	8	138	135	14 duplicate
16932	113	Galactose-6-phosphate	64	[789; Tyramine (3TMS)]	61	0.486	0.667	6.088	0.452	20	122	43	98	9	88 duplicate
12282	113	Galactose-6-phosphate	18	[590; 1-Acetyl-2-thiohydantoin]	62	0.486	0.631	9.007	0.426	21	120	48	94	30	106 duplicate
19038	113	Galactose-6-phosphate	100	[857; Mannitol (6TMS)]	62	0.486	0.578	10.466	0.442	22	121	55	87	39	93 duplicate
14835	113	Galactose-6-phosphate	41	[638; Proline (2TMS)]	62	0.485	0.648	14.826	0.521	23	119	45	97	68	63 duplicate
9549	113	Galactose-6-phosphate	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	62	0.483	0.904	32.239	0.573	24	118	5	137	125	32 original
19393	113	Galactose-6-phosphate	110	[715; Erythritol (4TMS)]	53	0.478	0.774	8.351	0.652	25	117	19	123	21	4 duplicate
14532	113	Galactose-6-phosphate	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	62	0.457	0.718	8.489	0.524	26	116	28	114	23	59 duplicate
19117	113	Galactose-6-phosphate	102	[904; Galactose methoxamine (5TMS)]	62	0.455	0.591	6.109	0.455	27	115	52	90	10	87 duplicate
11910	113	Galactose-6-phosphate	15	Alanine	62	0.450	0.740	19.073	0.542	28	114	24	118	85	51 duplicate
16777	113	Galactose-6-phosphate	62	[812; D-Xylofuranose (4TMS)]	62	0.436	0.790	15.489	0.562	29	113	15	127	74	45 duplicate
11784	113	Galactose-6-phosphate	14	Fumaric acid	62	0.433	0.679	5.944	0.442	30	112	39	103	7	92 duplicate
17647	113	Galactose-6-phosphate	74	[912; Tetradecanoic acid (1TMS)]	62	0.421	0.579	8.240	0.424	31	111	54	88	20	108 duplicate
13230	113	Galactose-6-phosphate	26	Citramalic acid	62	0.419	0.617	18.329	0.435	32	110	50	82	90	99 duplicate
18373	113	Galactose-6-phosphate	86	[793; D-Galactono-1,4-lactone (4TMS)]	59	0.419	0.859	19.801	0.593	33	109	7	135	99	16 duplicate
10740	113	Galactose-6-phosphate	6	Glycerol	62	0.413	0.822	43.280	0.563	34	108	12	130	141	43 duplicate
12645	113	Galactose-6-phosphate	21	[678; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	62	0.411	0.619	18.161	0.401	35	107	49	93	89	124 duplicate
9546	113	Galactose-6-phosphate	122	[644; Erythritol (4TMS)]	60	0.404	0.842	12.232	0.628	36	106	47	85	54	11 original
11400	113	Galactose-6-phosphate	11	Succinic acid	62	0.402	0.742	8.858	0.521	37	105	23	119	27	97 duplicate
12764	113	Galactose-6-phosphate	22	[690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.395	0.588	8.612	0.440	38	104	53	89	26	97 duplicate
19452	113	Galactose-6-phosphate	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	62	0.389	0.542	12.479	0.461	39	103	58	84	56	85 duplicate
9559	113	Galactose-6-phosphate	133	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	62	0.387	0.452	14.420	0.403	40	102	63	79	65	123 original
9557	113	Galactose-6-phosphate	133	[865; Squalene]	62	0.383	0.243	9.637	0.416	41	101	75	67	35	113 original
15129	113	Galactose-6-phosphate	44	[910; 2-Ketogluconic acid methoxamine (4TMS)]	49	0.367	0.688	7.974	0.647	42	100	35	107	19	5 duplicate
18480	113	Galactose-6-phosphate	88	Gluconic acid	62	0.358	0.678	11.953	0.584	43	99	40	102	48	22 duplicate
9562	113	Galactose-6-phosphate	138	[674; Ergosterol (1TMS)]	45	0.358	0.325	12.060	0.426	44	98	73	69	52	107 original
9550	113	Galactose-6-phosphate	126	[725; 2-Ketooctanoic acid (2TMS)]	62	0.357	0.723	33.343	0.588	45	97	27	115	130	19 duplicate
9556	113	Galactose-6-phosphate	132	[895; Isomaltose methoxamine (8TMS)]	42	0.354	0.578	12.803	0.494	46	96	56	88	59	74 original
14634	113	Galactose-6-phosphate	39	[828; 1-Phenylethanol (1TMS)]	45	0.354	0.671	6.365	0.657	47	95	42	100	11	3 original
13569	113	Galactose-6-phosphate	29	Erythritol	61	0.349	0.683	15.924	0.495	48	94	37	105	77	73 duplicate
18968	113	Galactose-6-phosphate	96	myo-Inositol	62	0.347	0.650	6.577	0.500	49	93	44	98	12	72 duplicate
12035	113	Galactose-6-phosphate	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	47	0.347	0.248	14.990	0.290	50	92	74	68	71	141 duplicate
19423	113	Galactose-6-phosphate	111	[583; Erythritol (4TMS)]	62	0.338	0.686	19.007	0.586	52	90	36	106	94	21 duplicate
16288	113	Galactose-6-phosphate	58	[929; Orotic acid (3TMS)]	42	0.324	0.443	16.990	0.421	53	89	65	77	82	109 duplicate
17008	113	Galactose-6-phosphate	65	[646; 3-Deoxyglucitol (5TMS)]	62	0.322	0.780	6.952	0.578	54	88	18	124	14	27 duplicate
15320	113	Galactose-6-phosphate	46	Arabinose	61	0.317	0.781	9.442	0.584	55	87	17	125	34	24 duplicate
12159	113	Galactose-6-phosphate	17	[700; 2-methyl-1,2-propanediol (2TMS)]	62	0.305	0.707	18.516	0.522	57	85	31	111	93	61 duplicate
9558	113	Galactose-6-phosphate	134	Isomaltose	62	0.304	0.767	25.193	0.576	58	84	20	122	115	29 original
11529	113	Galactose-6-phosphate	12	Glyceric acid	61	0.296	0.560	7.499	0.405	59	83	57	85	17	120 duplicate
17443	113	Galactose-6-phosphate	71	[731; Erythrose (3TMS)]	62	0.296	0.091	14.537	0.502	60	82	79	63	66	71 duplicate
9544	113	Galactose-6-phosphate	120	[945; Uridine (3TMS)]	54	0.282	0.172	12.647	0.449	61	81	77	65	58	90 original
19155	113	Galactose-6-phosphate	103	[648; Ethylamine (2TMS)]	61	0.278	0.505	14.037	0.512	62	80	61	81	64	68 duplicate
11657	113	Galactose-6-phosphate	13	Uracil	62	0.264	0.673	16.956	0.564	63	78	41	101	81	41 duplicate
19362	113	Galactose-6-phosphate	109	Octadecanoic acid	62	0.264	0.477	23.206	0.532	64	79	62	80	112	57 duplicate
8560	113	Galactose-6-phosphate	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.250	0.424	2.853	0.469	65	77	67	75	2	82 original

129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	58	0.234	0.706	9,328	0.569	66	76	32	110	33	36 original		
113	Galactose-6-phosphate	5580										76 duplicate		
50	[746; Ribonic acid-1,4-lactone (3TMS)]	59	0.225	0.592	14,033	0.490	67	75	51	91	63	38 duplicate		
113	Galactose-6-phosphate	18427										58 duplicate		
87	[945; beta-D-Glucopyranose (5TMS)]	60	0.198	0.728	35,605	0.568	68	74	25	117	134	138 original		
113	Galactose-6-phosphate	18028										78 duplicate		
140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	47	0.186	0.078	12,025	0.348	70	72	81	61	51	50 duplicate		
101	[832; Dopamine (4TMS)]	62	0.184	0.412	11,414	0.485	71	71	68	74	42	78 duplicate		
113	Galactose-6-phosphate	19078										51 duplicate		
92	[680; Glycerol-2-phosphate (4TMS)]	53	0.183	0.785	5,690	0.551	72	70	16	126	6	50 duplicate		
94	Hexadecanoic acid	62	0.169	0.351	23,226	0.536	73	69	70	72	113	54 duplicate		
113	Galactose-6-phosphate	18777										18 duplicate		
113	Galactose-6-phosphate	16044										95 original		
118	[928; Glucopyranose-6-phosphate (6TMS)]	58	0.165	0.378	7,723	0.441	75	67	69	73	18	33 duplicate		
113	Galactose-6-phosphate	18372										70 duplicate		
57	[757; 2-Deoxy-pentos-3-yose dimethoxyamine (2TMS)]	54	0.157	0.713	12,118	0.572	76	66	30	112	53	30 original		
91	[766; beta-D-Methylglucopyranoside (4TMS)]	62	0.117	0.328	17,488	0.502	77	65	72	70	86	105 duplicate		
128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.109	0.431	7,303	0.576	78	64	66	76	16	131 original		
113	Galactose-6-phosphate	16455										94 duplicate		
58	[636; 4R-Acetamid-2,3-(4Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	62	0.108	0.031	18,400	0.428	79	63	82	60	92	103 duplicate		
141	Lanosta-8,24-dien-3-beta-ol	59	0.094	-0.094	11,998	0.381	80	62	87	55	50	37 original		
36	[596; N-Acetylglutamic acid (2TMS)]	62	0.082	-0.100	30,830	0.441	81	61	88	54	122	49 duplicate		
7	Threonine	62	0.077	-0.102	32,308	0.430	82	60	89	53	126	89 original		
113	Galactose-6-phosphate	10874										104 duplicate		
137	Ergosterol	9561										37 original		
75	Lysine	17713										49 duplicate		
113	Galactose-6-phosphate	9551										53 duplicate		
127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	62	0.058	0.080	5,243	0.568	85	57	80	62	3	84 duplicate		
113	Galactose-6-phosphate	17157										108 duplicate		
67	Citic acid	9554										89 original		
113	Galactose-6-phosphate	16618										53 duplicate		
60	Glycerol-3-phosphate	9563										140 original		
113	Galactose-6-phosphate	17083										84 duplicate		
139	[700; Ergosta-5,7-dien-3-ol]	62	-0.002	-0.145	8,503	0.465	90	52	94	48	24	119 duplicate		
66	Glyceric acid-3-phosphate	124	[734; 1-Monocisglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	57	-0.025	-0.288	19,503	0.418	92	50	102	40	111 original	
2	Serine	62	-0.018	-0.162	21,760	0.408	91	51	95	47	108	77 duplicate		
113	Galactose-6-phosphate	14429										6 duplicate		
37	Phenylalanine	97	[756; beta-D-Methylglucopyranoside (4TMS)]	51	-0.053	0.345	20,520	0.646	94	48	71	104	35 duplicate	
113	Galactose-6-phosphate	18912										134 duplicate		
99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	-0.071	0.447	8,559	0.570	95	47	64	78	25	137 duplicate		
113	Galactose-6-phosphate	10489										117 duplicate		
4	Phosphoric acid	49	-0.112	-0.111	35,089	0.371	96	46	92	50	132	137 duplicate		
27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	51	-0.117	-0.447	19,181	0.361	97	45	117	25	98	137 duplicate		
9	Proline	61	-0.122	-0.223	30,325	0.410	98	44	99	43	121	117 duplicate		
31	[622; Parabanic acid (2TMS)]	62	-0.139	-0.356	10,878	0.397	99	43	106	36	41	125 duplicate		
113	Galactose-6-phosphate	19228										17 duplicate		
105	[705; 2-Ketogluconic acid (5TMS)]	47	-0.145	-0.106	12,455	0.593	100	42	91	51	55	69 duplicate		
84	Mannitol	60	-0.163	-0.048	34,285	0.508	101	41	84	58	131	2 duplicate		
113	Galactose-6-phosphate	18088										118 original		
119	[931; myo-Inositol-2-phosphate (7TMS)]	62	-0.173	-0.427	12,606	0.410	103	39	114	28	57	13 duplicate		
3	Ethanolamine	60	-0.180	-0.636	12,968	0.622	104	38	129	13	60	127 duplicate		
98	[897; Ribose-5-phosphate methoxyamine (5TMS)]	46	-0.186	-0.522	16,672	0.393	105	37	122	20	79	114 duplicate		
107	9-(Z)-Octadecanoic acid	62	-0.198	-0.492	17,743	0.414	106	36	120	22	88	135 duplicate		
8	Isoleucine	53	-0.200	-0.170	21,618	0.371	107	35	96	46	107	83 duplicate		
113	Galactose-6-phosphate	13898										100 duplicate		
32	[729; N,N-Dimethyllysine methyl ester]	61	-0.204	-0.409	17,719	0.468	108	34	112	30	87	112 duplicate		
72	[918; D-Xylopyranose (4TMS)]	61	-0.209	-0.267	11,423	0.433	109	33	101	41	43	80 duplicate		
113	Galactose-6-phosphate	43	[548; Leucine (2TBS)]	58	-0.214	-0.264	11,489	0.478	10	32	100	42	45	80 duplicate
23	Homoserine	62	-0.214	-0.538	15,375	0.417	111	31	124	18	73	112 duplicate		

17842	113 Galactose-6-phosphate	[826; beta-[(5-methyl-2-thenyl)methyleneamino-benzeneacetic acid methyl ester]	60	-0.215	-0.466	32.977	0.440	112	30	118	24	129	86 duplicate
15414	113 Galactose-6-phosphate	47 [NA]	62	-0.215	-0.092	13.477	0.513	113	29	88	56	61	67 duplicate
16537	113 Galactose-6-phosphate	59 Ornithine; Arginine	62	-0.217	-0.365	43.080	0.432	114	28	107	35	140	102 duplicate
18330	113 Galactose-6-phosphate	108 Octadecenoic acid	62	-0.241	-0.434	10.159	0.403	115	27	116	26	37	122 duplicate
18730	113 Galactose-6-phosphate	93 [607; Putrescine (4TMS)]	58	-0.246	-0.435	14.615	0.433	116	28	93	49	67	101 duplicate
14114	113 Galactose-6-phosphate	34 Aspartic acid	62	-0.248	-0.352	35.264	0.365	117	25	105	37	133	136 duplicate
14007	113 Galactose-6-phosphate	33 Methionine	62	-0.259	-0.409	14.948	0.373	118	24	111	31	89	133 duplicate
13880	113 Galactose-6-phosphate	30 [815; Ethyl-3(2H)-thiophenone]	62	-0.262	-0.372	32.696	0.384	119	23	109	33	127	128 duplicate
18983	113 Galactose-6-phosphate	80 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	62	-0.263	-0.427	11.463	0.420	120	22	113	29	44	110 duplicate
16698	113 Galactose-6-phosphate	81 [NA]	62	-0.283	-0.596	10.272	0.514	121	21	127	15	38	66 duplicate
17302	113 Galactose-6-phosphate	69 Arginine	58	-0.304	-0.576	25.249	0.493	122	20	125	17	117	75 duplicate
11270	113 Galactose-6-phosphate	10 Glycine	62	-0.306	-0.726	23.008	0.578	123	19	131	11	110	28 duplicate
15780	113 Galactose-6-phosphate	51 [498; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	62	-0.318	-0.531	17.323	0.384	124	18	123	19	85	129 duplicate
15957	113 Galactose-6-phosphate	53 Glycerol-2-phosphate	62	-0.320	-0.403	10.059	0.396	125	17	110	32	36	126 duplicate
15225	113 Galactose-6-phosphate	45 Homocysteine	59	-0.326	-0.510	18.337	0.382	126	16	121	21	81	130 duplicate
13115	113 Galactose-6-phosphate	25 [709; 2,5-Diaminovalerolactam (2TMS)]	47	-0.328	-0.479	15.897	0.532	127	15	119	23	76	56 duplicate
17230	113 Galactose-6-phosphate	68 [570; Hypoxanthine (2TMS)]	19	-0.333	-0.862	11.679	0.412	128	14	135	7	47	115 duplicate
15507	113 Galactose-6-phosphate	48 Asparagine	62	-0.338	-0.767	17.222	0.554	129	13	133	9	83	47 duplicate
14934	113 Galactose-6-phosphate	42 Glutamic acid	58	-0.355	-0.430	32.952	0.377	130	12	115	27	128	132 duplicate
10055	113 Galactose-6-phosphate	1 [938; Sulfuric acid (2TMS)]	35	-0.402	-0.220	8.861	0.645	131	11	88	44	28	7 duplicate
18823	113 Galactose-6-phosphate	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	41	-0.458	-0.727	16.773	0.478	132	10	132	10	80	79 duplicate
16130	113 Galactose-6-phosphate	55 [612; 4-Aminobutyric acid (2TBS)]	48	-0.458	-0.879	20.526	0.564	133	8	134	8	105	42 duplicate
9555	113 Galactose-6-phosphate	131 [626; 5-Methylthiodenosine (3TMS)]	53	-0.491	-0.796	15.137	0.593	134	8	134	8	72	15 original
15599	113 Galactose-6-phosphate	49 [877; Pyrophosphoric acid (4TMS)]	62	-0.519	-0.702	20.664	0.457	135	7	130	12	106	86 duplicate
10605	113 Galactose-6-phosphate	5 Leucine	43	-0.539	-0.598	13.912	0.411	136	6	128	14	62	118 duplicate
15669	113 Galactose-6-phosphate	52 [NA]	45	-0.554	-0.908	19.931	0.627	137	5	139	3	101	12 duplicate
18147	113 Galactose-6-phosphate	82 Lysine	37	-0.574	-0.887	22.559	0.630	138	4	138	4	109	10 duplicate
16855	113 Galactose-6-phosphate	63 Glutamine	51	-0.580	-0.879	20.367	0.553	139	3	137	5	103	48 duplicate
18532	113 Galactose-6-phosphate	89 [775; Dopamine (4TMS)]	34	-0.608	-0.945	20.099	0.582	140	2	141	1	102	25 duplicate
12525	113 Galactose-6-phosphate	20 [618; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	29	-0.700	-0.943	15.772	0.565	141	1	140	2	75	40 duplicate
19481	114 Fructose-6-phosphate	113 Galactose-6-phosphate	53	0.890	0.978	2.175	0.885	1	141	1	141	1	1 duplicate
9574	114 Fructose-6-phosphate	123 [945; Galactofuranose-6-phosphate (7TMS)]	53	0.801	0.914	11.441	0.659	2	140	3	139	53	4 original
9568	114 Fructose-6-phosphate	115 Glucose-6-phosphate	53	0.758	0.958	25.444	0.619	3	139	2	140	118	15 original
12405	114 Fructose-6-phosphate	19 Alanine (BP) (3TMS)	53	0.668	0.845	12.169	0.565	4	138	8	134	58	45 duplicate
14221	114 Fructose-6-phosphate	35 Pyrogutamic acid	53	0.618	0.909	40.980	0.616	5	137	4	138	140	18 duplicate
17581	114 Fructose-6-phosphate	73 [708; Glucose methoxyamine (5TMS)]	46	0.586	0.785	6.062	0.524	6	136	12	130	10	64 duplicate
17668	114 Fructose-6-phosphate	79 Glucose	53	0.586	0.889	33.730	0.598	7	135	5	137	133	25 duplicate
18206	114 Fructose-6-phosphate	83 Sorbitol	47	0.584	0.161	21.893	0.383	8	134	77	65	111	127 duplicate
13458	114 Fructose-6-phosphate	28 Malic acid	53	0.570	0.770	11.203	0.529	9	133	15	127	51	63 duplicate
14838	114 Fructose-6-phosphate	41 [639; Proline (2TMS)]	53	0.567	0.701	14.617	0.552	10	132	31	111	74	55 duplicate
19193	114 Fructose-6-phosphate	104 [795; Erythritol (4TMS)]	52	0.557	0.703	6.917	0.577	11	131	30	112	16	37 duplicate
19039	114 Fructose-6-phosphate	100 [857; Mannitol (6TMS)]	53	0.554	0.675	11.049	0.504	12	130	38	104	49	79 duplicate
9567	114 Fructose-6-phosphate	116 [982; Pseudouridine (5TMS)]	28	0.540	0.318	7.290	0.443	13	129	74	68	119	100 original
17779	114 Fructose-6-phosphate	76 Fructose	53	0.536	0.886	25.610	0.561	14	128	6	136	119	34 duplicate
18319	114 Fructose-6-phosphate	85 [529; Methylcitric acid (4TMS)]	37	0.535	0.862	6.641	0.441	15	127	41	101	14	101 duplicate
17906	114 Fructose-6-phosphate	78 Mannose	51	0.523	0.808	6.019	0.566	16	126	10	132	9	44 duplicate
17648	114 Fructose-6-phosphate	74 [912; Tetradecanoic acid (1TMS)]	53	0.517	0.697	7.719	0.475	17	125	32	110	24	85 duplicate
16933	114 Fructose-6-phosphate	64 [789; Tyramine (3TMS)]	53	0.512	0.714	6.152	0.449	18	124	27	115	12	97 duplicate
9572	114 Fructose-6-phosphate	121 [657; Erythritol (4TMS)]	46	0.511	0.764	7.010	0.587	19	123	17	125	18	32 original

11911	114	Fructose-6-phosphate	15	Alanine	53	0.507	0.752	18,175	0.537	20	122	20	122	94	60 duplicate
19264	114	Fructose-6-phosphate	106	[733; Threitol (4TMS)]	53	0.504	0.808	10,259	0.634	21	121	11	131	44	9 duplicate
9568	114	Fructose-6-phosphate	117	[724; Glycerol (3TMS)]	48	0.496	0.767	5,830	0.591	22	120	16	126	8	30 original
12283	114	Fructose-6-phosphate	18	[590; 1-Acetyl-2-thiohydantoin]	53	0.491	0.644	9,488	0.429	23	119	47	95	35	103 duplicate
14736	114	Fructose-6-phosphate	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	53	0.486	0.746	34,982	0.554	24	118	23	119	137	53 duplicate
19118	114	Fructose-6-phosphate	102	[904; Galactose methoxamine (5TMS)]	53	0.485	0.673	5,722	0.522	25	117	40	102	7	67 duplicate
9576	114	Fructose-6-phosphate	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	53	0.463	0.865	31,328	0.603	26	116	7	135	129	23 original
17374	114	Fructose-6-phosphate	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	46	0.463	0.722	18,751	0.517	27	115	25	117	101	69 duplicate
11785	114	Fructose-6-phosphate	14	Fumaric acid	53	0.460	0.720	4,612	0.510	28	114	26	116	4	74 duplicate
13231	114	Fructose-6-phosphate	26	Citramalic acid	53	0.458	0.631	18,245	0.456	29	113	52	90	97	95 duplicate
9589	114	Fructose-6-phosphate	138	[674; Ergosterol (1TMS)]	41	0.439	0.543	10,107	0.505	30	112	62	80	42	78 original
9584	114	Fructose-6-phosphate	133	[855; Squalene]	53	0.435	0.428	8,588	0.416	31	111	67	75	28	106 original
19394	114	Fructose-6-phosphate	110	[715; Erythritol (4TMS)]	45	0.432	0.775	7,599	0.683	32	110	14	128	22	2 duplicate
12646	114	Fructose-6-phosphate	21	[678; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	53	0.415	0.635	18,386	0.389	33	109	50	92	98	124 duplicate
12765	114	Fructose-6-phosphate	22	[690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	45	0.408	0.648	6,063	0.465	34	108	45	97	11	89 duplicate
18689	114	Fructose-6-phosphate	96	myo-Inositol	40	0.390	0.425	12,476	0.346	35	107	68	74	59	133 duplicate
19453	114	Fructose-6-phosphate	112	[677; beta-D-Galactopyranoside-(1,2)-glycerol (8TMS)]	53	0.389	0.596	10,003	0.483	36	106	58	84	40	82 duplicate
9573	114	Fructose-6-phosphate	122	[644; Erythritol (4TMS)]	43	0.382	0.636	9,299	0.622	37	105	49	93	33	13 original
16778	114	Fructose-6-phosphate	62	[812; D-Xylofuranose (4TMS)]	53	0.382	0.775	15,762	0.571	38	103	13	129	80	40 duplicate
14533	114	Fructose-6-phosphate	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	53	0.382	0.704	9,444	0.535	39	104	29	113	34	61 duplicate
11401	114	Fructose-6-phosphate	11	Succinic acid	53	0.377	0.711	9,555	0.534	40	102	28	114	38	62 duplicate
9586	114	Fructose-6-phosphate	135	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	53	0.376	0.511	14,567	0.398	41	101	64	78	73	120 original
10741	114	Fructose-6-phosphate	6	Glycerol	53	0.370	0.753	41,360	0.548	43	99	19	123	141	57 duplicate
9583	114	Fructose-6-phosphate	132	[895; Isomaltose methoxamine (8TMS)]	40	0.346	0.603	10,525	0.487	44	98	57	85	46	81 original
9591	114	Fructose-6-phosphate	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	42	0.336	0.354	9,833	0.406	45	97	71	71	38	113 original
18374	114	Fructose-6-phosphate	86	[793; D-Galactono-1,4-lactone (4TMS)]	50	0.324	0.816	21,031	0.608	46	96	9	133	108	19 duplicate
19363	114	Fructose-6-phosphate	109	Octadecanoic acid	53	0.319	0.588	23,388	0.517	47	95	59	83	115	70 duplicate
19424	114	Fructose-6-phosphate	111	[583; Erythritol (4TMS)]	41	0.302	0.526	15,323	0.444	48	94	63	79	78	89 duplicate
9577	114	Fructose-6-phosphate	126	[559; Erythritol (4TMS)]	40	0.297	0.615	5,265	0.648	49	93	56	86	5	6 original
11530	114	Fructose-6-phosphate	12	Glyceric acid	52	0.287	0.579	5,579	0.456	50	92	60	82	6	94 duplicate
17444	114	Fructose-6-phosphate	71	[731; Erythrose (3TMS)]	53	0.274	0.135	14,508	0.473	51	91	79	63	72	87 duplicate
15130	114	Fructose-6-phosphate	44	[910; 2-Ketogluconic acid methoxamine (4TMS)]	41	0.271	0.623	8,820	0.825	52	90	53	89	29	11 duplicate
13000	114	Fructose-6-phosphate	24	[725; 2-Ketooctanoic acid (2TMS)]	53	0.267	0.684	33,117	0.605	53	88	36	106	131	20 duplicate
13570	114	Fructose-6-phosphate	29	Erythritol	53	0.267	0.617	6,910	0.513	54	89	54	88	15	71 duplicate
18481	114	Fructose-6-phosphate	88	Gluconic acid	53	0.266	0.644	13,108	0.592	55	87	46	96	61	29 duplicate
9571	114	Fructose-6-phosphate	120	[945; Uridine (3TMS)]	48	0.261	0.137	13,666	0.449	56	86	78	64	67	96 original
12036	114	Fructose-6-phosphate	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	53	0.257	0.852	19,659	0.604	57	85	44	98	104	21 duplicate
14635	114	Fructose-6-phosphate	39	[829; 1-Phenylethanol (1TMS)]	52	0.256	0.684	17,324	0.559	58	84	35	107	90	50 duplicate
16289	114	Fructose-6-phosphate	56	[829; Ornic acid (3TMS)]	53	0.254	0.749	7,590	0.627	59	83	22	120	21	10 duplicate
18778	114	Fructose-6-phosphate	94	Hexadecanoic acid	53	0.247	0.499	22,954	0.523	60	82	65	77	112	66 duplicate
18029	114	Fructose-6-phosphate	80	[772; D-Glucose (5TMS)]	51	0.242	0.633	29,355	0.510	61	81	51	91	123	72 duplicate
19156	114	Fructose-6-phosphate	103	[646; Ethylamine (2TMS)]	53	0.235	0.458	15,266	0.507	62	80	68	76	76	78 duplicate
12160	114	Fructose-6-phosphate	17	[700; 2-methyl-1,2-propanediol (2TMS)]	53	0.231	0.668	19,464	0.570	63	79	42	100	103	41 duplicate
9569	114	Fructose-6-phosphate	118	[928; Glucopyranose-6-phosphate (6TMS)]	51	0.227	0.392	7,506	0.464	64	78	72	70	20	90 original
9587	114	Fructose-6-phosphate	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.221	0.392	2,888	0.461	65	77	70	72	2	91 original
17009	114	Fructose-6-phosphate	65	[646; 3-Deoxyglucitol (5TMS)]	52	0.211	0.749	10,055	0.640	66	76	21	121	41	8 duplicate
11658	114	Fructose-6-phosphate	13	Uracil	53	0.209	0.852	17,907	0.604	67	75	43	99	93	22 duplicate
15321	114	Fructose-6-phosphate	46	Arabinose	53	0.205	0.756	17,452	0.618	68	74	18	124	91	16 duplicate
9585	114	Fructose-6-phosphate	134	Isomaltose	53	0.202	0.733	26,114	0.596	69	73	24	118	120	27 original
18428	114	Fructose-6-phosphate	87	[945; beta-D-Glucopyranose (5TMS)]	51	0.200	0.673	33,828	0.561	70	72	39	103	134	48 duplicate

9592	114	Fructose-6-phosphate	141	Lanosta-8,24-dien-3 $\beta$ -ol	50	0.180	0.115	9.055	0.411	71	71	81	61	32	108	original
9590	114	Fructose-6-phosphate	139	[700; Ergosta-5,7-dien-3-ol]	34	0.180	0.131	13.226	0.392	72	70	80	62	63	121	original
15691	114	Fructose-6-phosphate	50	[746; Ribonic acid-1,4-lactone (3TMS)]	52	0.173	0.570	11.273	0.509	73	69	61	81	52	75	duplicate
9580	114	Fructose-6-phosphate	129	[840; Maltose methoxamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	51	0.153	0.685	10.255	0.620	74	68	34	108	43	14	original
16456	114	Fructose-6-phosphate	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	53	0.151	0.089	17.128	0.405	75	67	82	60	88	114	duplicate
18079	114	Fructose-6-phosphate	101	[832; Dopamine (4TMS)]	53	0.141	0.319	12.395	0.470	76	66	73	69	58	88	duplicate
9598	114	Fructose-6-phosphate	137	Ergosterol	53	0.135	0.031	16.600	0.351	77	65	85	57	85	131	original
18634	114	Fructose-6-phosphate	91	[766; beta-D-Methylglucopyranoside (4TMS)]	53	0.122	0.261	18.223	0.550	78	64	75	67	96	56	duplicate
17714	114	Fructose-6-phosphate	75	Lysine	53	0.112	0.041	38.784	0.409	79	63	84	58	138	110	duplicate
16045	114	Fructose-6-phosphate	54	[NA]	46	0.109	0.644	6.927	0.554	80	62	48	94	17	54	duplicate
14326	114	Fructose-6-phosphate	36	[596; N-Acetylglutamic acid (2TMS)]	53	0.094	-0.038	29.063	0.415	81	61	89	53	122	107	duplicate
9591	114	Fructose-6-phosphate	130	Trehalose	53	0.093	0.001	30.336	0.409	82	60	87	55	126	111	original
10875	114	Fructose-6-phosphate	7	Threonine	53	0.081	-0.052	30.795	0.402	83	58	90	52	128	117	duplicate
16619	114	Fructose-6-phosphate	60	Glycerol-3-phosphate	53	0.081	-0.191	23.287	0.554	84	59	98	44	113	52	duplicate
16373	114	Fructose-6-phosphate	57	[757; 2-Desoxy-pentose-3-yose dimethoxamine (2TMS)]	47	0.073	0.680	13.377	0.567	85	57	37	105	66	43	duplicate
18663	114	Fructose-6-phosphate	92	[680; Glycerol-2-phosphate (4TMS)]	45	0.071	0.892	6.552	0.561	86	56	33	108	13	35	duplicate
9578	114	Fructose-6-phosphate	127	[777; Fructose-6-phosphate methoxamine (8TMS)]	37	0.066	0.059	4.466	0.562	87	55	83	59	3	47	original
8575	114	Fructose-6-phosphate	124	[734; 1-Monoolcylglycerol (2TMS); 1-Monohexadecenylglycerol (1TMS)]	48	0.023	-0.086	16.450	0.438	88	54	91	51	84	102	original
17158	114	Fructose-6-phosphate	67	Clitic acid	53	0.012	-0.286	25.344	0.510	89	53	104	38	117	73	duplicate
17084	114	Fructose-6-phosphate	66	Glyceric acid-3-phosphate	53	-0.013	-0.161	7.763	0.524	90	52	95	47	25	65	duplicate
10470	114	Fructose-6-phosphate	4	Phosphoric acid	4	-0.033	-0.035	32.089	0.300	91	51	88	54	130	141	duplicate
10195	114	Fructose-6-phosphate	2	Serine	51	-0.037	-0.121	19.961	0.384	92	50	93	49	105	128	duplicate
9579	114	Fructose-6-phosphate	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	40	-0.038	0.002	8.433	0.585	93	48	86	56	26	33	original
14430	114	Fructose-6-phosphate	37	Phenylalanine	53	-0.051	-0.254	24.341	0.496	94	48	101	41	116	80	duplicate
11140	114	Fructose-6-phosphate	9	Proline	52	-0.118	-0.173	27.828	0.377	95	47	97	45	121	129	duplicate
18913	114	Fructose-6-phosphate	97	[756; beta-D-Methylglucopyranoside (4TMS)]	44	-0.118	0.246	21.716	0.642	96	46	76	66	110	7	duplicate
18089	114	Fructose-6-phosphate	81	Tyrosine	53	-0.120	-0.522	34.830	0.649	97	45	122	20	136	5	duplicate
10333	114	Fructose-6-phosphate	3	Elhandamine	51	-0.125	-0.577	11.521	0.817	98	44	126	16	54	17	duplicate
18998	114	Fructose-6-phosphate	99	[662; Ribose-5-phosphate methoxamine (BP) (5TMS)]	40	-0.126	0.399	7.608	0.557	99	43	69	73	23	51	duplicate
17513	114	Fructose-6-phosphate	72	[919; D-Xylopyranose (4TMS)]	40	-0.148	-0.269	10.374	0.459	100	42	102	40	45	93	duplicate
18538	114	Fructose-6-phosphate	59	Omithine; Arginine	52	-0.173	-0.317	40.502	0.404	101	41	107	35	139	115	duplicate
19288	114	Fructose-6-phosphate	107	9-(Z)-Octadecanoic acid	53	-0.174	-0.332	17.080	0.385	102	40	109	33	87	125	duplicate
17843	114	Fructose-6-phosphate	77	benzeneacetic acid methyl ester	51	-0.178	-0.405	30.623	0.448	103	39	117	25	127	98	duplicate
13791	114	Fructose-6-phosphate	31	[622; Parabenic acid (2TMS)]	53	-0.183	-0.384	9.777	0.402	104	38	114	28	37	118	duplicate
13900	114	Fructose-6-phosphate	32	[728; N,N-Dimethyllysine methyl ester]	52	-0.187	-0.395	16.329	0.478	105	37	116	26	83	84	duplicate
13345	114	Fructose-6-phosphate	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	42	-0.192	-0.514	18.197	0.328	106	38	121	21	95	139	duplicate
9570	114	Fructose-6-phosphate	119	[931; myo-Inositol-2-phosphate (7TMS)]	53	-0.202	-0.315	11.687	0.410	107	35	106	36	55	109	original
18263	114	Fructose-6-phosphate	84	Mannitol	51	-0.208	-0.104	34.175	0.546	108	34	92	50	135	58	duplicate
15415	114	Fructose-6-phosphate	47	[NA]	53	-0.209	-0.168	13.138	0.589	109	33	86	46	62	31	duplicate
11008	114	Fructose-6-phosphate	8	Isoleucine	44	-0.214	-0.137	20.068	0.305	110	32	94	48	106	140	duplicate
19331	114	Fructose-6-phosphate	108	Octadecanoic acid	53	-0.218	-0.315	8.824	0.402	111	30	105	37	30	119	duplicate
14008	114	Fructose-6-phosphate	33	Methionine	53	-0.218	-0.368	13.840	0.335	112	31	113	29	68	136	duplicate
13681	114	Fructose-6-phosphate	30	[815; Ethyl-3(2H)-thiophenone]	53	-0.232	-0.327	30.331	0.341	113	29	108	34	125	135	duplicate
18584	114	Fructose-6-phosphate	90	[910; 9-(Z)-Hexadecanoic acid (1TMS)]	53	-0.234	-0.280	10.677	0.403	114	28	103	39	47	116	duplicate
12883	114	Fructose-6-phosphate	23	Homoserine	53	-0.261	-0.584	14.137	0.424	115	27	127	15	70	105	duplicate
15033	114	Fructose-6-phosphate	43	[548; Leucine (2TBS)]	49	-0.269	-0.344	11.173	0.480	116	26	110	32	50	83	duplicate

14115	114	Fructose-6-phosphate	34	Aspartic acid	53	-0.271	-0.360	33.226	0.331	117	25	112	30	132	137 duplicate
11271	114	Fructose-6-phosphate	10	Glycine	53	-0.279	-0.706	21.691	0.593	118	24	131	11	109	28 duplicate
19229	114	Fructose-6-phosphate	105	[705; 2-Ketogluconic acid (5TMS)]	40	-0.285	-0.353	13.315	0.576	119	23	111	31	65	38 duplicate
14935	114	Fructose-6-phosphate	42	Glutamic acid	49	-0.286	-0.389	29.810	0.330	120	22	115	27	124	138 duplicate
17303	114	Fructose-6-phosphate	69	Arginine	49	-0.287	-0.575	23.361	0.520	121	21	125	17	114	68 duplicate
18958	114	Fructose-6-phosphate	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	37	-0.306	-0.623	15.276	0.392	122	20	129	13	77	123 duplicate
15958	114	Fructose-6-phosphate	53	Glycerol-2-phosphate	53	-0.313	-0.418	8.531	0.360	123	19	118	24	27	128 duplicate
18731	114	Fructose-6-phosphate	93	Glycerol-2-phosphate	50	-0.319	-0.209	12.343	0.427	124	18	99	43	57	104 duplicate
16699	114	Fructose-6-phosphate	61	[NA]	53	-0.324	-0.564	9.872	0.505	125	17	124	18	39	77 duplicate
15226	114	Fructose-6-phosphate	45	Homocysteine	50	-0.326	-0.511	15.982	0.348	126	16	120	22	81	132 duplicate
15781	114	Fructose-6-phosphate	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	35	-0.341	-0.543	15.687	0.359	127	15	123	19	79	130 duplicate
13116	114	Fructose-6-phosphate	25	[708; 2,5-Diaminovalerolactam (2TMS)]	42	-0.366	-0.477	15.018	0.564	128	14	119	23	75	48 duplicate
10056	114	Fructose-6-phosphate	1	[938; Sulfuric acid (2TMS)]	34	-0.378	-0.239	8.932	0.663	129	13	100	42	31	3 duplicate
15508	114	Fructose-6-phosphate	48	Asparagine	53	-0.379	-0.792	18.207	0.561	130	12	133	9	82	48 duplicate
18148	114	Fructose-6-phosphate	82	Lysine	53	-0.448	-0.877	20.803	0.600	131	11	138	4	107	24 duplicate
18131	114	Fructose-6-phosphate	55	[612; 4-Aminobutyric acid (2TBS)]	33	-0.466	-0.875	17.816	0.539	132	10	137	5	92	59 duplicate
17231	114	Fructose-6-phosphate	68	[570; Hypoxanthine (2TMS)]	18	-0.477	-0.837	10.922	0.392	133	9	135	7	48	122 duplicate
18824	114	Fructose-6-phosphate	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	39	-0.517	-0.753	14.117	0.474	134	8	132	10	69	86 duplicate
15600	114	Fructose-6-phosphate	49	[877; Pyrophosphoric acid (4TMS)]	53	-0.522	-0.686	18.697	0.460	135	7	130	12	100	92 duplicate
10608	114	Fructose-6-phosphate	5	Leucine	34	-0.554	-0.815	12.980	0.345	136	6	128	14	60	134 duplicate
9582	114	Fructose-6-phosphate	131	[626; 5-Methylthioadenosine (3TMS)]	44	-0.575	-0.824	13.265	0.597	137	5	134	8	64	26 original
15870	114	Fructose-6-phosphate	52	[NA]	40	-0.618	-0.904	17.217	0.624	138	4	139	3	89	12 duplicate
18533	114	Fructose-6-phosphate	89	[775; Dopamine (4TMS)]	30	-0.623	-0.923	18.583	0.568	139	3	141	1	99	42 duplicate
18658	114	Fructose-6-phosphate	63	Glutamine	48	-0.640	-0.864	18.906	0.578	140	2	136	6	102	38 duplicate
12526	114	Fructose-6-phosphate	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxethylamine (4TMS)]	24	-0.645	-0.923	14.336	0.574	141	1	140	2	71	39 duplicate
14222	115	Glucose-6-phosphate	35	Pyroglutamic acid	62	0.760	0.957	17.275	0.632	1	141	4	138	46	20 duplicate
18509	115	Glucose-6-phosphate	114	Fructose-6-phosphate	53	0.758	0.958	25.444	0.619	2	140	3	139	95	26 duplicate
17780	115	Glucose-6-phosphate	76	Fructose	62	0.741	0.964	4.875	0.651	3	139	2	140	1	11 duplicate
19482	115	Glucose-6-phosphate	113	Galactose-6-phosphate	62	0.739	0.967	25.551	0.571	4	138	1	141	98	53 duplicate
13459	115	Glucose-6-phosphate	28	Malic acid	62	0.731	0.834	16.978	0.588	5	137	21	121	45	43 duplicate
19395	115	Glucose-6-phosphate	110	[715; Erythritol (4TMS)]	53	0.701	0.892	26.973	0.648	6	136	8	134	106	12 duplicate
9594	115	Glucose-6-phosphate	117	[724; Glycerol (3TMS)]	56	0.697	0.788	24.144	0.686	7	135	36	106	87	45 original
14737	115	Glucose-6-phosphate	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	62	0.695	0.827	11.802	0.589	8	134	25	117	23	42 duplicate
9598	115	Glucose-6-phosphate	121	[657; Erythritol (4TMS)]	53	0.694	0.816	31.812	0.590	9	133	31	111	118	41 original
19040	115	Glucose-6-phosphate	100	[857; Mannitol (6TMS)]	62	0.692	0.681	17.766	0.584	10	132	51	91	47	47 duplicate
19265	115	Glucose-6-phosphate	106	[733; Threitol (4TMS)]	61	0.686	0.889	18.824	0.626	11	131	11	131	56	25 duplicate
9599	115	Glucose-6-phosphate	122	[844; Erythritol (4TMS)]	50	0.657	0.826	32.585	0.630	12	130	28	116	121	22 original
9603	115	Glucose-6-phosphate	126	[559; Erythritol (4TMS)]	45	0.644	0.833	25.049	0.653	13	129	23	119	93	10 original
11786	115	Glucose-6-phosphate	14	Fumaric acid	62	0.644	0.809	28.120	0.575	14	128	35	107	108	50 duplicate
17907	115	Glucose-6-phosphate	78	Mannose	60	0.643	0.867	25.695	0.573	15	127	14	128	99	51 duplicate
15131	115	Glucose-6-phosphate	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	49	0.643	0.827	20.461	0.639	16	126	24	118	69	18 duplicate
14534	115	Glucose-6-phosphate	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	62	0.640	0.836	19.169	0.601	17	125	20	122	59	36 duplicate
17582	115	Glucose-6-phosphate	73	[708; Glucose methoxyamine (5TMS)]	55	0.618	0.840	23.868	0.506	18	124	19	123	86	75 duplicate
19119	115	Glucose-6-phosphate	102	[904; Galactose methoxyamine (5TMS)]	62	0.617	0.665	25.085	0.571	19	123	53	89	94	54 duplicate
16779	115	Glucose-6-phosphate	62	[812; D-Xylofuranose (4TMS)]	62	0.611	0.868	11.689	0.603	20	122	13	129	21	34 duplicate
12766	115	Glucose-6-phosphate	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.609	0.749	28.906	0.582	21	121	43	99	111	48 duplicate
11402	115	Glucose-6-phosphate	11	Succinic acid	62	0.602	0.833	18.892	0.590	22	120	22	120	55	40 duplicate
18375	115	Glucose-6-phosphate	86	[783; D-Galactono-1,4-lactone (4TMS)]	59	0.592	0.833	15.558	0.665	23	119	5	137	39	4 duplicate
13232	115	Glucose-6-phosphate	26	Citramelic acid	62	0.575	0.714	10.267	0.506	24	118	46	96	16	76 duplicate
12647	115	Glucose-6-phosphate	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	62	0.568	0.698	9.797	0.537	25	117	48	94	12	64 duplicate

9609	115 Glucose-6-phosphate	132 [895; Isomaltose methoxyamine (8TMS)]	42 0.568	0.762	30.590	0.610	28	116	41	101	113	30 original
17375	115 Glucose-6-phosphate	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	55 0.566	0.731	7.495	0.472	27	115	45	97	2	89 duplicate
13001	115 Glucose-6-phosphate	24 [725; 2-Ketocacetic acid (2TMS)]	62 0.557	0.844	8.532	0.861	28	114	17	125	6	7 duplicate
12284	115 Glucose-6-phosphate	18 [590; 1-Acetyl-2-thiohydantoin]	62 0.555	0.638	19.363	0.478	28	113	58	84	60	87 duplicate
12037	115 Glucose-6-phosphate	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	62 0.548	0.816	8.425	0.640	30	112	30	112	4	17 duplicate
9602	115 Glucose-6-phosphate	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	62 0.543	0.911	8.265	0.607	31	111	6	136	3	32 original
19454	115 Glucose-6-phosphate	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	62 0.542	0.822	36.705	0.522	32	110	62	80	134	72 duplicate
14838	115 Glucose-6-phosphate	39 [829; 1-Phenylethanol (1TMS)]	61 0.541	0.821	14.824	0.603	33	109	27	115	30	35 duplicate
16290	115 Glucose-6-phosphate	56 [829; Orolic acid (3TMS)]	62 0.537	0.890	25.542	0.683	34	108	10	132	97	1 duplicate
13571	115 Glucose-6-phosphate	29 Erythritol	62 0.535	0.776	23.045	0.596	35	107	40	102	79	38 duplicate
17649	115 Glucose-6-phosphate	74 [912; Tetradecanoic acid (1TMS)]	62 0.533	0.640	24.724	0.454	36	108	58	86	88	99 duplicate
12406	115 Glucose-6-phosphate	19 Alanine (BP) (3TMS)	62 0.530	0.815	14.838	0.527	37	104	32	110	34	68 duplicate
18482	115 Glucose-6-phosphate	88 Gluconic acid	62 0.530	0.788	16.791	0.628	38	105	37	105	44	24 duplicate
9600	115 Glucose-6-phosphate	123 [945; Galactofuranose-6-phosphate (7TMS)]	62 0.528	0.782	15.520	0.520	39	103	38	104	38	73 original
17010	115 Glucose-6-phosphate	65 [646; 3-Deoxyglucitol (5TMS)]	61 0.520	0.892	25.524	0.672	40	102	9	133	96	2 duplicate
18320	115 Glucose-6-phosphate	85 [529; Methylcitric acid (4TMS)]	46 0.519	0.642	18.026	0.402	41	101	55	87	57	123 duplicate
15322	115 Glucose-6-phosphate	46 Arabinose	62 0.511	0.900	15.933	0.658	42	99	7	135	40	9 duplicate
9612	115 Glucose-6-phosphate	135 [902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	62 0.508	0.523	14.334	0.483	44	98	66	76	28	84 original
9611	115 Glucose-6-phosphate	134 Isomaltose	62 0.504	0.879	8.877	0.861	45	97	12	130	7	6 original
11531	115 Glucose-6-phosphate	12 Glycemic acid	61 0.504	0.691	30.317	0.557	46	96	49	93	112	56 duplicate
8959	115 Glucose-6-phosphate	116 [882; Pseudouridine (5TMS)]	30 0.494	0.257	20.246	0.465	47	95	78	66	87	93 original
11659	115 Glucose-6-phosphate	13 Uracil	62 0.487	0.813	11.157	0.629	48	94	33	109	19	23 duplicate
12161	115 Glucose-6-phosphate	17 [700; 2-methyl-1,2-propanediol (2TMS)]	62 0.484	0.816	9.132	0.573	49	93	29	113	8	52 duplicate
19157	115 Glucose-6-phosphate	103 [648; Ethylamine (2TMS)]	61 0.478	0.646	20.114	0.552	50	92	54	88	65	59 duplicate
9806	115 Glucose-6-phosphate	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	58 0.466	0.843	23.228	0.637	51	91	18	124	81	19 original
9597	115 Glucose-6-phosphate	Glc]	54 0.458	0.225	14.800	0.570	52	90	78	64	33	55 original
18684	115 Glucose-6-phosphate	92 [680; Glyceral-2-phosphate (4TMS)]	53 0.451	0.850	23.217	0.612	53	89	16	126	80	28 duplicate
15692	115 Glucose-6-phosphate	50 [748; Ribonic acid-1,4-lactone (3TMS)]	59 0.449	0.741	37.958	0.551	54	88	44	98	137	61 duplicate
18637	115 Glucose-6-phosphate	41 [639; Proline (2TMS)]	62 0.439	0.639	13.009	0.473	55	87	57	85	28	88 duplicate
19194	115 Glucose-6-phosphate	104 [795; Erythritol (4TMS)]	61 0.438	0.672	21.894	0.505	56	86	52	90	75	77 duplicate
18207	115 Glucose-6-phosphate	83 Sorbitol	56 0.434	-0.002	11.507	0.307	57	85	84	58	20	138 duplicate
16046	115 Glucose-6-phosphate	54 [NA]	54 0.427	0.780	29.075	0.618	58	84	39	103	109	27 duplicate
16374	115 Glucose-6-phosphate	57 [757; 2-Deoxy-pentose-3-yose dimethoxyamine (2TMS)]	54 0.423	0.859	18.797	0.664	59	83	15	127	63	5 duplicate
9605	115 Glucose-6-phosphate	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45 0.420	0.705	19.116	0.659	60	82	47	95	58	8 original
10742	115 Glucose-6-phosphate	6 Glycerol	62 0.393	0.818	18.146	0.534	61	81	28	114	52	65 duplicate
19080	115 Glucose-6-phosphate	101 [832; Dopamine (4TMS)]	62 0.377	0.534	21.278	0.490	62	80	65	77	73	83 duplicate
9604	115 Glucose-6-phosphate	127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	39 0.368	0.465	21.264	0.668	63	79	69	73	72	3 original
18870	115 Glucose-6-phosphate	96 myo-Inositol	47 0.367	0.251	36.099	0.292	64	78	77	65	133	139 duplicate
9815	115 Glucose-6-phosphate	138 [674; Ergosterol (1TMS)]	45 0.345	0.305	32.658	0.411	65	77	75	67	122	121 original
19425	115 Glucose-6-phosphate	111 [583; Erythritol (4TMS)]	42 0.340	0.473	37.736	0.468	66	76	68	74	136	90 duplicate
18635	115 Glucose-6-phosphate	91 [766; beta-D-Methylglucopyranoside (4TMS)]	62 0.310	0.461	23.486	0.454	67	75	70	72	84	98 duplicate
19364	115 Glucose-6-phosphate	109 Octadecanoic acid	62 0.299	0.498	12.442	0.500	68	74	67	75	24	79 duplicate
17969	115 Glucose-6-phosphate	79 Glucose	62 0.293	0.810	11.105	0.584	69	73	34	108	18	46 duplicate
16934	115 Glucose-6-phosphate	64 [789; Tyramine (3TMS)]	61 0.293	0.569	23.766	0.441	70	72	63	79	85	106 duplicate
9817	115 Glucose-6-phosphate	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	47 0.286	0.180	32.369	0.448	71	71	80	62	120	101 original
9810	115 Glucose-6-phosphate	133 [855; Squalene]	62 0.279	0.218	22.223	0.340	72	70	79	63	76	137 original
18429	115 Glucose-6-phosphate	87 [945; beta-D-Glucopyranose (5TMS)]	60 0.276	0.760	12.659	0.545	73	69	42	100	25	63 duplicate
11912	115 Glucose-6-phosphate	15 Alanine	62 0.269	0.638	9.385	0.611	74	68	59	83	10	29 duplicate

9613	115 Glucose-6-phosphate	136 [748; D-Scdheptulose-7-phosphate (7TMS)]	17	0.265	0.437	14,630	0.530	75	67	71	71	31	67 original
18914	115 Glucose-6-phosphate	97 [756; beta-D-Methylglucopyranoside (4TMS)]	51	0.255	0.544	15,973	0.576	76	68	64	78	41	49 duplicate
19230	115 Glucose-6-phosphate	105 [705; 2-Keiogluconic acid (5TMS)]	47	0.234	0.384	20,235	0.630	77	65	72	70	68	21 duplicate
18779	115 Glucose-6-phosphate	94 Hexadecanoic acid	62	0.231	0.378	9,759	0.503	78	64	73	69	11	78 duplicate
18030	115 Glucose-6-phosphate	80 [772; D-Glucose (5TMS)]	60	0.211	0.685	9,960	0.513	79	63	50	92	14	74 duplicate
9618	115 Glucose-6-phosphate	141 Lancoside-8,24-dien-3-beta-ol	59	0.175	-0.003	32,966	0.476	80	62	85	57	123	86 original
17445	115 Glucose-6-phosphate	71 [731; Erythrose (3TMS)]	62	0.106	-0.009	15,025	0.419	81	61	86	58	37	116 duplicate
9614	115 Glucose-6-phosphate	137 Ergosterol	62	0.106	-0.090	18,072	0.439	82	60	88	54	51	108 original
9595	115 Glucose-6-phosphate	118 [928; Glucopyranose-6-phosphate (6TMS)]	58	0.082	0.319	26,407	0.525	83	59	74	68	101	69 original
9616	115 Glucose-6-phosphate	139 [700; Ergosta-5,7-dien-3-ol]	37	0.075	-0.153	33,755	0.450	84	58	90	52	124	100 original
18999	115 Glucose-6-phosphate	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	0.024	0.632	26,886	0.642	85	57	60	82	104	15 duplicate
18264	115 Glucose-6-phosphate	84 Mannitol	60	0.011	0.118	14,437	0.418	86	56	81	61	29	118 duplicate
9601	115 Glucose-6-phosphate	124 [734; 1-Monoolleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]	57	-0.019	-0.281	42,823	0.461	87	55	98	44	140	94 original
9596	115 Glucose-6-phosphate	119 [931; myo-Inositol-2-phosphate (7TMS)]	62	-0.024	-0.317	22,552	0.495	88	54	101	41	77	81 original
18732	115 Glucose-6-phosphate	93 [607; Putrescine (4TMS)]	58	-0.041	0.018	35,521	0.418	89	53	82	60	130	117 duplicate
15416	115 Glucose-6-phosphate	47 [NA]	62	-0.051	-0.013	24,743	0.477	90	52	87	55	89	85 duplicate
18457	115 Glucose-6-phosphate	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	62	-0.079	-0.114	14,927	0.346	91	51	88	53	35	136 duplicate
10876	115 Glucose-6-phosphate	7 Threonine	62	-0.102	-0.238	10,432	0.364	92	50	94	48	17	135 duplicate
19299	115 Glucose-6-phosphate	107 9-(Z)-Octadecanoic acid	62	-0.104	-0.413	14,067	0.443	93	49	107	35	27	104 duplicate
18595	115 Glucose-6-phosphate	90 [910; 9-(Z)-Hexadecanoic acid (1TMS)]	62	-0.105	-0.290	21,860	0.436	94	48	99	43	74	111 duplicate
17715	115 Glucose-6-phosphate	75 Lysine	62	-0.108	-0.193	18,001	0.368	95	47	92	50	60	129 duplicate
14327	115 Glucose-6-phosphate	36 [596; N-Acetylglutamic acid (2TMS)]	62	-0.118	-0.259	11,709	0.377	96	46	96	46	22	134 duplicate
9607	115 Glucose-6-phosphate	130 Trehalose	61	-0.136	-0.184	9,802	0.394	97	45	91	51	13	127 original
16620	115 Glucose-6-phosphate	67 Glycerol-3-phosphate	62	-0.155	-0.382	10,205	0.461	98	44	106	38	15	95 duplicate
17159	115 Glucose-6-phosphate	60 Citric acid	62	-0.169	-0.466	8,462	0.416	99	43	110	32	5	120 duplicate
10196	115 Glucose-6-phosphate	2 Serine	60	-0.173	-0.303	20,362	0.382	100	42	100	42	68	132 duplicate
10471	115 Glucose-6-phosphate	4 Phosphoric acid	49	-0.179	-0.195	14,632	0.288	101	41	93	49	32	140 duplicate
17085	115 Glucose-6-phosphate	66 Glyceralic acid-3-phosphate	62	-0.195	-0.321	26,031	0.433	102	40	102	40	100	112 duplicate
15959	115 Glucose-6-phosphate	53 Glycerol-2-phosphate	62	-0.203	-0.333	31,129	0.392	103	39	104	38	116	128 duplicate
17514	115 Glucose-6-phosphate	72 [919; D-Xylopyranose (4TMS)]	61	-0.215	-0.253	27,557	0.380	104	38	95	47	107	133 duplicate
14431	115 Glucose-6-phosphate	37 Phenylalanine	62	-0.236	-0.447	9,144	0.422	105	37	108	34	9	114 duplicate
13346	115 Glucose-6-phosphate	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	51	-0.274	-0.592	35,101	0.444	106	36	119	23	128	103 duplicate
19332	115 Glucose-6-phosphate	108 Octadecanoic acid	62	-0.282	-0.465	26,916	0.397	107	35	109	33	105	126 duplicate
11141	115 Glucose-6-phosphate	9 Proline	61	-0.294	-0.368	19,756	0.402	108	34	105	37	62	124 duplicate
11009	115 Glucose-6-phosphate	8 Isoleucine	53	-0.300	-0.279	17,959	0.287	109	33	97	45	48	141 duplicate
13792	115 Glucose-6-phosphate	31 [622; Parabenic acid (2TMS)]	62	-0.326	-0.492	30,832	0.443	110	32	112	30	114	105 duplicate
15034	115 Glucose-6-phosphate	43 [548; Leucine (2TBS)]	58	-0.327	-0.330	21,028	0.405	111	31	103	39	71	122 duplicate
10057	115 Glucose-6-phosphate	1 [938; Sulfuric acid (2TMS)]	35	-0.328	0.001	22,640	0.646	112	30	83	59	78	14 duplicate
10334	115 Glucose-6-phosphate	3 Ethanolamine	60	-0.349	-0.724	30,944	0.554	113	29	130	12	115	57 duplicate
15871	115 Glucose-6-phosphate	52 [NA]	45	-0.376	-0.856	35,760	0.588	114	28	135	7	131	44 duplicate
16700	115 Glucose-6-phosphate	61 [NA]	62	-0.377	-0.627	23,254	0.494	115	27	121	21	82	82 duplicate
13901	115 Glucose-6-phosphate	32 [729; N,N-Dimethyllysine methyl ester]	61	-0.384	-0.573	34,147	0.523	116	26	118	24	125	71 duplicate
18090	115 Glucose-6-phosphate	81 Tyrosine	62	-0.387	-0.708	18,488	0.598	117	25	127	15	53	37 duplicate
18957	115 Glucose-6-phosphate	98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	46	-0.389	-0.666	35,474	0.447	118	24	123	19	129	102 duplicate
17232	115 Glucose-6-phosphate	68 [570; Hypoxanthine (2TMS)]	19	-0.392	-0.905	23,391	0.466	119	23	138	4	83	92 duplicate
	115 Glucose-6-phosphate	[826; beta-[[[5-methyl-2-thenyl)methyleneamino-benzeneacetic acid methyl ester]	60	-0.400	-0.593	18,642	0.418	120	22	120	22	54	119 duplicate
17044	115 Glucose-6-phosphate	34 Aspartic acid	62	-0.401	-0.472	14,929	0.438	121	21	111	31	36	109 duplicate
14116	115 Glucose-6-phosphate	23 Homoserine	62	-0.406	-0.679	24,944	0.531	122	20	125	17	82	68 duplicate



16539	115 Glucose-6-phosphate	59 Ornithine; Arginine	62 -0.407	-0.496	19.845	0.437	123	19	113	29	64	110 duplicate
14009	115 Glucose-6-phosphate	33 Methionine	62 -0.412	-0.524	24.750	0.458	124	18	115	27	90	96 duplicate
13682	115 Glucose-6-phosphate	30 [815; Ethyl-3-(2H)-thiophenone]	62 -0.434	-0.502	16.226	0.384	125	17	114	28	42	130 duplicate
15227	115 Glucose-6-phosphate	45 Homocysteine	59 -0.452	-0.566	41.204	0.383	126	16	117	25	139	131 duplicate
15782	115 Glucose-6-phosphate	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	43 -0.453	-0.645	35.375	0.422	127	15	122	20	128	115 duplicate
17304	115 Glucose-6-phosphate	69 Arginine	58 -0.471	-0.709	17.971	0.552	128	14	128	14	49	58 duplicate
18825	115 Glucose-6-phosphate	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	48 -0.477	-0.748	35.872	0.441	129	13	131	11	132	107 duplicate
15509	115 Glucose-6-phosphate	48 Asparagine	62 -0.481	-0.835	26.629	0.592	130	12	133	9	103	39 duplicate
11272	115 Glucose-6-phosphate	10 Glycine	62 -0.491	-0.840	16.233	0.641	131	11	134	8	43	16 duplicate
16132	115 Glucose-6-phosphate	55 [612; 4-Aminobutyric acid (2BTS)]	41 -0.507	-0.890	37.089	0.497	132	10	137	5	135	80 duplicate
14938	115 Glucose-6-phosphate	42 Glutamic acid	58 -0.514	-0.866	20.932	0.425	133	9	116	26	70	113 duplicate
16857	115 Glucose-6-phosphate	63 Glutamine	51 -0.515	-0.863	32.014	0.647	134	8	136	8	119	13 duplicate
18534	115 Glucose-6-phosphate	89 [775; Dopamine (4TMS)]	34 -0.526	-0.944	29.211	0.524	135	7	140	2	110	70 duplicate
10607	115 Glucose-6-phosphate	5 Leucine	43 -0.539	-0.879	24.922	0.397	136	6	124	18	91	125 duplicate
15601	115 Glucose-6-phosphate	49 [877; Pyrophosphoric acid (4TMS)]	62 -0.575	-0.694	40.400	0.455	137	5	128	16	138	97 duplicate
13117	115 Glucose-6-phosphate	25 [709; 2,5-Diaminovalerolactam (2TMS)]	47 -0.576	-0.712	31.788	0.608	138	4	129	13	117	31 duplicate
18149	115 Glucose-6-phosphate	82 Lysine	37 -0.598	-0.924	19.408	0.604	139	3	139	3	61	33 duplicate
9608	115 Glucose-6-phosphate	131 [626; 5-Methylthioadenosine (3TMS)]	53 -0.668	-0.828	35.270	0.551	140	2	132	10	127	62 original
12527		20 [618; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	29 -0.670	-0.955	26.627	0.551	141	1	141	1	102	60 duplicate
18780	116 [882; Pseudouridine (5T	94 Hexadecanoic acid	30 0.720	0.767	19.671	0.435	1	140	6	135	115	61 duplicate
9637	116 [882; Pseudouridine (5T		30 0.692	0.777	11.914	0.345	2	139	5	138	68	111 original
19455	116 [882; Pseudouridine (5T	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	30 0.687	0.712	9.634	0.402	3	138	9	132	48	79 duplicate
9640	116 [882; Pseudouridine (5T	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	27 0.687	0.682	8.365	0.472	4	137	14	127	27	30 original
9834	116 [882; Pseudouridine (5T	[674; Ergosterol (1TMS)]	20 0.674	0.699	7.713	0.439	5	136	10	131	19	57 original
18365	116 [882; Pseudouridine (5T	[895; Isomaltose methoxyamine (8TMS)]	30 0.674	0.681	21.492	0.467	6	135	15	126	120	33 duplicate
9643	116 [882; Pseudouridine (5T	Octadecanoic acid	30 0.637	0.792	6.085	0.528	7	133	3	138	4	7 original
9639	116 [882; Pseudouridine (5T	[141 Lanosta-8,24-dien-3-beta-ol	30 0.637	0.789	13.176	0.550	8	134	4	137	86	4 original
12767	116 [882; Pseudouridine (5T	[137 Ergosterol	25 0.627	0.643	7.072	0.322	9	132	18	123	12	119 duplicate
9642	116 [882; Pseudouridine (5T	[690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	29 0.606	0.633	9.382	0.456	10	131	21	120	42	41 original
19120	116 [882; Pseudouridine (5T	[692; Ergosta-7,22-dien-3-ol (1TMS)]	30 0.605	0.570	6.986	0.442	11	130	29	112	9	55 duplicate
17650	116 [882; Pseudouridine (5T	[904; Galactose methoxyamine (5TMS)]	30 0.563	0.629	8.292	0.372	12	129	22	119	25	98 duplicate
9635	116 [882; Pseudouridine (5T	[912; Tetradecanoic acid (1TMS)]	30 0.549	0.450	8.784	0.387	13	128	43	98	33	88 original
17446	116 [882; Pseudouridine (5T	[855; Squalene]	30 0.545	0.798	12.527	0.503	14	126	2	139	78	19 duplicate
18041	116 [882; Pseudouridine (5T	[731; Erythrose (3TMS)]	30 0.545	0.664	9.430	0.409	15	127	16	125	44	74 duplicate
19426	116 [882; Pseudouridine (5T	[857; Mannitol (6TMS)]	23 0.542	0.660	12.523	0.382	16	125	17	124	77	89 duplicate
18510	116 [882; Pseudouridine (5T	[583; Erythritol (4TMS)]	28 0.540	0.318	7.290	0.443	17	124	60	81	14	54 duplicate
18871	116 [882; Pseudouridine (5T	Fructose-6-phosphate	29 0.532	0.738	12.342	0.272	18	123	8	133	73	133 duplicate
18321	116 [882; Pseudouridine (5T	myo-Inositol	30 0.531	0.565	7.710	0.324	19	122	31	110	18	118 duplicate
13233	116 [882; Pseudouridine (5T	[529; Methylcitric acid (4TMS)]	30 0.526	0.600	14.468	0.316	20	121	25	116	98	122 duplicate
18208	116 [882; Pseudouridine (5T	Citramalic acid	30 0.517	0.578	19.508	0.485	21	119	28	113	113	27 duplicate
19483	116 [882; Pseudouridine (5T	Sorbitol	30 0.517	0.179	9.030	0.446	22	120	78	63	37	50 duplicate
18047	116 [882; Pseudouridine (5T	Galactose-6-phosphate	25 0.500	0.368	8.627	0.362	23	118	53	88	31	102 duplicate
18536	116 [882; Pseudouridine (5T	[NA]	30 0.494	0.257	20.246	0.465	24	117	68	73	118	78 duplicate
11532	116 [882; Pseudouridine (5T	Glucose-6-phosphate	30 0.485	0.640	7.010	0.404	25	116	20	121	11	37 duplicate
13460	116 [882; Pseudouridine (5T	Glyceric acid	30 0.476	0.538	9.771	0.451	26	115	32	109	51	45 duplicate
11403	116 [882; Pseudouridine (5T	Malic acid	30 0.467	0.477	8.711	0.310	27	114	41	100	32	124 duplicate
11787	116 [882; Pseudouridine (5T	Succinic acid	30 0.457	0.502	6.949	0.404	28	113	36	105	8	77 duplicate
9625	116 [882; Pseudouridine (5T	Fumaric acid	30 0.444	0.221	11.358	0.501	29	112	76	65	62	20 original
12407	116 [882; Pseudouridine (5T	[945; Galactofuranose-6-phosphate (7TMS)]	30 0.425	0.223	12.374	0.339	30	111	75	66	74	112 duplicate

9641	116 [882; Pseudouridine (5T 139 [700; Ergosta-5,7-dien-3-ol]	22	0,420	0,454	12,304	0,428	31	110	42	99	71	65 original
14223	116 [882; Pseudouridine (5T 35 Pyroglutamic acid	30	0,411	0,202	31,053	0,503	32	109	77	64	137	17 duplicate
14838	116 [882; Pseudouridine (5T 41 [639; Proline (2TMS)]	30	0,402	0,255	13,460	0,293	33	108	70	71	90	128 duplicate
16780	116 [882; Pseudouridine (5T 62 [812; D-Xylofuranose (4TMS)]	30	0,389	0,241	12,775	0,445	34	107	71	70	80	52 duplicate
17376	116 [882; Pseudouridine (5T 70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	28	0,365	0,177	14,782	0,298	35	106	79	62	100	128 duplicate
12285	116 [882; Pseudouridine (5T 18 [590; 1-Acetyl-2-thiohydantoin]	30	0,347	0,373	9,362	0,357	36	105	52	89	41	107 duplicate
	124 [734; 1-Monodeoxyglycerol (2TMS); 1-											
9626	116 [882; Pseudouridine (5T Monohexadecenylglycerol (1TMS)]	30	0,338	0,601	13,340	0,503	37	104	24	117	87	16 original
14738	116 [882; Pseudouridine (5T 40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	30	0,315	0,504	26,592	0,407	38	103	35	106	133	76 duplicate
16621	116 [882; Pseudouridine (5T 60 Glycero-3-phosphate	30	0,310	0,524	18,998	0,458	39	101	34	107	111	42 duplicate
14535	116 [882; Pseudouridine (5T 38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	30	0,310	0,488	8,618	0,377	40	102	40	101	29	94 duplicate
13572	116 [882; Pseudouridine (5T 29 Erythritol	30	0,301	0,501	7,470	0,317	41	100	37	104	15	121 duplicate
9627	116 [882; Pseudouridine (5T 125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	30	0,297	0,037	24,079	0,366	42	99	90	51	125	100 original
12648	116 [882; Pseudouridine (5T 21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	30	0,292	0,381	14,391	0,507	43	98	60	91	97	13 duplicate
18483	116 [882; Pseudouridine (5T 88 Gluconic acid	30	0,287	0,349	9,960	0,459	44	97	55	86	52	40 duplicate
18685	116 [882; Pseudouridine (5T 92 [680; Glycerol-2-phosphate (4TMS)]	24	0,275	0,099	9,714	0,387	45	96	83	58	47	85 duplicate
16935	116 [882; Pseudouridine (5T 64 [788; Tyramine (3TMS)]	30	0,269	-0,029	8,279	0,280	46	95	97	44	24	131 duplicate
16375	57 [757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	26	0,268	0,313	11,560	0,407	47	94	61	80	66	75 duplicate
9630	116 [882; Pseudouridine (5T 128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	19	0,263	0,683	6,904	0,446	48	93	13	128	7	49 original
11660	116 [882; Pseudouridine (5T 13 Uracil	30	0,260	0,396	12,799	0,418	49	91	48	93	81	71 duplicate
17908	116 [882; Pseudouridine (5T 78 Mannose	30	0,260	0,267	9,760	0,485	50	92	66	75	50	28 duplicate
9629	116 [882; Pseudouridine (5T 127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	18	0,255	0,754	3,808	0,470	51	90	7	134	2	31 original
9623	116 [882; Pseudouridine (5T 121 [657; Erythritol (4TMS)]	24	0,254	0,588	8,620	0,464	52	89	30	111	6	38 original
15693	116 [882; Pseudouridine (5T 746; Ribonic acid-1,4-lactone (3TMS)]	29	0,246	0,414	11,318	0,257	53	88	47	94	61	134 duplicate
12038	116 [882; Pseudouridine (5T 50 [644; 2-Methyl-1,3-butanediol (2TMS)]	30	0,241	0,420	14,380	0,426	54	87	46	95	96	67 duplicate
17011	116 [882; Pseudouridine (5T 65 [646; 3-Deoxyglucitol (2TMS)]	30	0,237	0,348	10,394	0,494	55	86	56	85	58	22 duplicate
19398	116 [882; Pseudouridine (5T 110 [745; Erythritol (4TMS)]	23	0,233	0,622	8,131	0,609	56	85	23	118	23	1 duplicate
16291	116 [882; Pseudouridine (5T 56 [828; Orotic acid (3TMS)]	30	0,232	0,289	9,198	0,466	57	84	62	79	39	34 duplicate
13002	116 [882; Pseudouridine (5T 24 [725; 2-Ketocacanic acid (2TMS)]	30	0,228	0,375	23,837	0,453	58	83	51	90	123	44 duplicate
9622	116 [882; Pseudouridine (5T 120 [845; Uridine (3TMS)]	27	0,225	0,077	11,861	0,292	59	82	88	53	67	129 original
14637	116 [882; Pseudouridine (5T 39 [829; 1-Phenylethanol (1TMS)]	30	0,223	0,430	12,501	0,417	60	81	45	96	76	72 duplicate
9628	116 [882; Pseudouridine (5T 119 [559; Erythritol (4TMS)]	20	0,211	0,906	5,921	0,567	61	80	1	140	3	2 original
9621	116 [882; Pseudouridine (5T 119 [931; myo-Inositol-2-phosphate (7TMS)]	30	0,209	0,698	8,334	0,438	62	77	11	130	26	58 original
12162	116 [882; Pseudouridine (5T 17 [700; 2-methyl-1,2-propanediol (2TMS)]	30	0,209	0,383	14,020	0,351	63	78	49	92	94	109 duplicate
15323	116 [882; Pseudouridine (5T 46 Arabinose	30	0,209	0,267	13,484	0,483	64	79	65	76	92	28 duplicate
19300	116 [882; Pseudouridine (5T 107 9-(Z)-Octadecenoic acid	30	0,205	0,526	13,112	0,381	65	78	33	108	85	92 duplicate
	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-											
	Glc											
9631	116 [882; Pseudouridine (5T Glc	29	0,192	0,364	9,472	0,451	66	75	54	87	45	47 original
19158	116 [882; Pseudouridine (5T 103 [648; Ethylamine (2TMS)]	30	0,191	0,269	9,729	0,375	67	73	64	77	49	96 duplicate
11913	116 [882; Pseudouridine (5T 15 Alanine	30	0,191	-0,270	16,168	0,420	68	74	113	28	104	69 duplicate
18826	116 [882; Pseudouridine (5T 95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	18	0,190	0,266	8,008	0,362	69	72	67	74	20	101 duplicate
9636	116 [882; Pseudouridine (5T 134 Isomaltose	30	0,186	0,329	18,224	0,474	70	71	58	83	110	29 original
17583	116 [882; Pseudouridine (5T 73 [708; Glucose methoxyamine (5TMS)]	30	0,182	0,322	9,337	0,386	71	70	59	82	40	87 duplicate
17781	116 [882; Pseudouridine (5T 76 Fructose	30	0,177	0,233	20,719	0,508	72	69	72	69	119	14 duplicate
8819	116 [882; Pseudouridine (5T 117 [724; Glycerol (3TMS)]	26	0,175	0,493	7,679	0,505	73	68	38	103	17	15 original
18586	116 [882; Pseudouridine (5T 90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	30	0,172	0,486	8,112	0,359	74	65	39	102	22	104 duplicate
19266	116 [882; Pseudouridine (5T 106 [733; Threitol (4TMS)]	30	0,172	0,331	11,484	0,520	75	66	57	84	64	8 duplicate
18376	116 [882; Pseudouridine (5T 86 [793; D-Galactono-1,4-lactone (4TMS)]	30	0,172	0,228	17,576	0,512	76	67	73	68	108	11 duplicate
9620	116 [882; Pseudouridine (5T 118 [928; Glucopyranose-6-phosphate (6TMS)]	29	0,158	-0,154	10,419	0,358	77	64	108	35	57	105 original
19195	116 [882; Pseudouridine (5T 104 [795; Erythritol (4TMS)]	30	0,136	0,115	10,103	0,392	78	62	82	59	54	82 duplicate

10877	116 [882; Pseudouridine (5T 7	Threonine	30	0.136	0.084	24.545	0.468	79	83	87	54	127	32 duplicate
19000	116 [882; Pseudouridine (5T 99	[862; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	22	0.134	0.541	7.084	0.389	80	61	19	122	13	84 duplicate
9624	116 [882; Pseudouridine (5T 122	[644; Erythritol (4TMS)]	22	0.126	0.598	6.990	0.558	81	60	26	115	10	3 original
9638	116 [882; Pseudouridine (5T 136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	13	0.103	0.228	2.463	0.382	82	59	74	67	1	91 original
18430	116 [882; Pseudouridine (5T 87	[945; beta-D-Glucopyranose (5TMS)]	30	0.090	-0.027	26.400	0.313	83	58	96	45	132	123 duplicate
18915	116 [882; Pseudouridine (5T 97	[756; beta-D-Methylglucopyranoside (4TMS)]	24	0.087	0.029	12.841	0.376	84	57	91	50	83	95 duplicate
19081	116 [882; Pseudouridine (5T 101	[832; Dopamine (4TMS)]	30	0.085	0.091	8.019	0.410	85	56	85	56	38	73 duplicate
15132	116 [882; Pseudouridine (5T 44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	21	0.076	0.687	9.716	0.515	86	55	12	129	48	10 duplicate
17160	116 [882; Pseudouridine (5T 67	Citric acid	30	0.071	0.434	20.054	0.465	87	54	44	97	117	36 duplicate
19231	116 [882; Pseudouridine (5T 105	[705; 2-Ketogluconic acid (5TMS)]	20	0.053	0.584	7.618	0.435	88	53	27	114	16	62 duplicate
10058	116 [882; Pseudouridine (5T 1	[938; Sulfuric acid (2TMS)]	17	0.044	0.280	6.580	0.534	89	52	63	78	5	6 duplicate
14432	116 [882; Pseudouridine (5T 37	Phenylalanine	30	0.044	0.094	18.584	0.449	90	48	84	57	114	48 duplicate
18636	116 [882; Pseudouridine (5T 91	[766; beta-D-Methylglucopyranoside (4TMS)]	30	0.044	-0.020	10.007	0.492	91	49	85	46	53	23 duplicate
17970	116 [882; Pseudouridine (5T 79	Glucose	30	0.044	-0.113	26.940	0.437	92	50	101	40	134	59 duplicate
10743	116 [882; Pseudouridine (5T 6	Glycerol	30	0.044	-0.140	31.507	0.194	93	51	104	37	139	138 duplicate
18031	116 [882; Pseudouridine (5T 80	[772; D-Glucose (5TMS)]	28	0.037	-0.162	23.032	0.248	94	47	107	34	121	136 duplicate
15672	116 [882; Pseudouridine (5T 52	[NA]	20	0.032	0.256	11.157	0.351	95	46	69	72	60	110 duplicate
19333	116 [882; Pseudouridine (5T 108	Octadecanoic acid	30	0.021	0.089	8.047	0.337	96	45	86	55	21	114 duplicate
17515	116 [882; Pseudouridine (5T 72	[918; D-Xylopyranose (4TMS)]	30	0.002	-0.259	10.209	0.429	97	44	111	30	55	63 duplicate
18265	116 [882; Pseudouridine (5T 84	Mannitol	28	-0.021	0.158	18.496	0.441	98	43	80	61	112	56 duplicate
9632	116 [882; Pseudouridine (5T 130	Trehalose	30	-0.053	-0.071	23.634	0.427	99	42	100	41	122	66 original
16701	116 [882; Pseudouridine (5T 61	[NA]	30	-0.090	-0.014	8.928	0.303	100	40	94	47	34	125 duplicate
17716	116 [882; Pseudouridine (5T 75	Lysine	30	-0.090	-0.376	31.204	0.489	101	41	127	14	138	24 duplicate
16458	116 [882; Pseudouridine (5T	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	30	-0.108	-0.413	15.412	0.508	102	39	131	10	101	12 duplicate
10335	116 [882; Pseudouridine (5T 3	Ethanolamine	29	-0.108	0.054	8.469	0.444	103	38	89	52	28	53 duplicate
10472	116 [882; Pseudouridine (5T 4	Phosphoric acid	30	-0.117	-0.430	28.792	0.358	104	37	134	7	135	106 duplicate
12528	116 [882; Pseudouridine (5T		18	-0.124	0.017	11.482	0.429	105	36	92	49	63	64 duplicate
18091	116 [882; Pseudouridine (5T 81	Tyrosine	30	-0.136	-0.055	28.803	0.465	106	35	89	42	136	35 duplicate
17233	116 [882; Pseudouridine (5T 68	[570; Hypoxanthine (2TMS)]	12	-0.152	-0.424	9.017	0.284	107	34	132	9	35	130 duplicate
16133	116 [882; Pseudouridine (5T 55	[612; 4-Aminobutyric acid (2TBS)]	24	-0.152	-0.043	14.360	0.331	108	33	98	43	95	116 duplicate
18733	116 [882; Pseudouridine (5T 93	[607; Putrescine (4TMS)]	29	-0.158	0.147	10.760	0.518	109	32	81	60	58	9 duplicate
15783	116 [882; Pseudouridine (5T 51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	23	-0.162	-0.185	12.987	0.179	110	31	108	33	84	139 duplicate
13683	116 [882; Pseudouridine (5T 30	[615; Ethyl-3(2H)-thiophenone]	30	-0.172	-0.273	24.726	0.390	111	30	114	27	128	83 duplicate
15417	116 [882; Pseudouridine (5T 47	[NA]	30	-0.195	-0.400	11.515	0.459	112	29	130	11	65	39 duplicate
17845	116 [882; Pseudouridine (5T	[626; beta-[[[5-methyl-2-phenyl(methyl)amino]- benzeneacetic acid methyl ester]	30	-0.200	-0.115	25.824	0.383	113	28	102	39	130	88 duplicate
14328	116 [882; Pseudouridine (5T 36	[596; N-Acetylglutamic acid (2TMS)]	30	-0.214	-0.231	24.381	0.500	114	27	109	32	126	21 duplicate
14010	116 [882; Pseudouridine (5T 33	Methionine	30	-0.218	-0.273	12.474	0.334	115	26	115	26	75	115 duplicate
10608	116 [882; Pseudouridine (5T 5	Leucine	27	-0.219	-0.378	12.335	0.172	116	25	128	13	72	140 duplicate
14937	116 [882; Pseudouridine (5T 42	Glutamic acid	28	-0.227	-0.298	25.310	0.360	117	24	117	24	129	103 duplicate
10197	116 [882; Pseudouridine (5T 2	Serine	30	-0.237	-0.441	17.042	0.485	118	23	135	6	107	25 duplicate
13902	116 [882; Pseudouridine (5T 32	[729; N,N-Dimethyllysine methyl ester]	30	-0.241	-0.346	12.223	0.367	119	21	122	19	69	99 duplicate
11142	116 [882; Pseudouridine (5T 9	Proline	30	-0.241	-0.392	23.933	0.503	120	22	129	12	124	18 duplicate
15228	116 [882; Pseudouridine (5T 45	Homocysteine	27	-0.254	-0.288	13.973	0.252	121	20	116	25	93	135 duplicate
11010	116 [882; Pseudouridine (5T 8	Isoleucine	30	-0.255	-0.302	16.825	0.399	122	19	118	23	105	80 duplicate
14117	116 [882; Pseudouridine (5T 34	Aspartic acid	30	-0.260	-0.269	26.333	0.325	123	17	112	29	131	117 duplicate
17305	116 [882; Pseudouridine (5T 69	Arginine	30	-0.260	-0.348	19.711	0.420	124	18	123	18	116	70 duplicate
15960	116 [882; Pseudouridine (5T 53	Glycerol-2-phosphate	30	-0.269	-0.149	9.188	0.297	125	16	105	36	38	127 duplicate
18150	116 [882; Pseudouridine (5T 82	Lysine	27	-0.299	-0.326	15.731	0.423	126	15	121	20	103	68 duplicate

18535	116 [882; Pseudouridine (5T 89 [775; Dopamine (4TMS)]	23 -0.304	-0.007	14,544	0.436	127	14	93	48	98	60 duplicate
15510	116 [882; Pseudouridine (5T 48 Asparagine	30 -0.315	-0.232	13,389	0.396	128	12	110	31	89	81 duplicate
15602	116 [882; Pseudouridine (5T 49 [877; Pyrophosphoric acid (4TMS)]	30 -0.315	-0.367	17,000	0.382	129	13	125	16	106	90 duplicate
16540	116 [882; Pseudouridine (5T 59 Ornithine; Arginine	30 -0.324	-0.317	32,030	0.451	130	10	119	22	140	48 duplicate
13793	116 [882; Pseudouridine (5T 31 [622; Parabenic acid (2TMS)]	30 -0.324	-0.351	9,427	0.338	131	11	124	17	43	113 duplicate
11273	116 [882; Pseudouridine (5T 10 Glycine	30 -0.358	-0.317	17,830	0.445	132	9	120	21	109	51 duplicate
9633	116 [882; Pseudouridine (5T 131 [626; 5-Methylthioadenosine (3TMS)]	24 -0.384	-0.428	12,251	0.375	133	8	133	8	70	97 original
12885	116 [882; Pseudouridine (5T 23 Homoserine	30 -0.430	-0.547	13,382	0.355	134	7	139	2	88	108 duplicate
16958	116 [882; Pseudouridine (5T 63 Glutamine	27 -0.430	-0.138	12,814	0.378	135	6	103	38	82	93 duplicate
17006	116 [882; Pseudouridine (5T 66 Glycine acid-3-phosphate	30 -0.457	-0.371	8,624	0.455	136	5	126	15	30	43 duplicate
15035	116 [882; Pseudouridine (5T 48 [548; Leucine (2TBS)]	28 -0.508	-0.513	10,791	0.320	137	4	136	5	59	120 duplicate
13347	116 [882; Pseudouridine (5T 27 [915; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	26 -0.514	-0.545	15,590	0.243	138	3	137	4	102	137 duplicate
13118	116 [882; Pseudouridine (5T 25 [709; 2,5-Diaminovalerolactam (2TMS)]	20 -0.516	-0.546	13,472	0.538	139	2	138	3	91	5 duplicate
18958	116 [882; Pseudouridine (5T 98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	19 -0.520	-0.559	12,682	0.278	140	1	140	1	79	132 duplicate
19397	117 [724; Glycerol (3TMS)]	52 0.916	0.948	5,412	0.670	1	141	5	137	6	4 duplicate
9647	117 [724; Glycerol (3TMS)]	50 0.886	0.962	8,905	0.673	2	140	2	140	30	3 original
9648	117 [724; Glycerol (3TMS)]	48 0.883	0.971	9,182	0.695	3	139	1	141	31	1 original
15133	117 [724; Glycerol (3TMS)]	47 0.856	0.953	4,271	0.641	4	138	3	139	2	6 duplicate
19267	117 [724; Glycerol (3TMS)]	55 0.857	0.944	6,647	0.690	5	137	6	136	12	2 duplicate
9652	117 [724; Glycerol (3TMS)]	44 0.793	0.953	3,884	0.661	6	136	4	138	1	5 original
17782	117 [724; Glycerol (3TMS)]	56 0.757	0.812	24,239	0.606	7	135	12	130	120	9 duplicate
14739	117 [724; Glycerol (3TMS)]	56 0.701	0.884	33,167	0.586	8	134	7	135	135	23 duplicate
19537	117 [724; Glycerol (3TMS)]	56 0.697	0.788	24,144	0.586	9	133	16	126	119	22 duplicate
14224	117 [724; Glycerol (3TMS)]	56 0.649	0.757	39,815	0.593	10	132	26	116	140	18 duplicate
17909	117 [724; Glycerol (3TMS)]	54 0.628	0.811	5,532	0.563	11	131	13	129	7	25 duplicate
19042	117 [724; Glycerol (3TMS)]	56 0.609	0.773	9,398	0.571	12	130	23	119	33	34 duplicate
13461	117 [724; Glycerol (3TMS)]	56 0.604	0.858	9,491	0.563	13	129	8	134	34	37 duplicate
17684	117 [724; Glycerol (3TMS)]	49 0.573	0.790	5,394	0.473	14	128	18	124	5	93 duplicate
11788	117 [724; Glycerol (3TMS)]	56 0.561	0.822	6,890	0.578	15	127	11	131	16	30 duplicate
14638	117 [724; Glycerol (3TMS)]	56 0.553	0.838	13,810	0.602	16	126	9	133	64	12 duplicate
12768	117 [724; Glycerol (3TMS)]	49 0.532	0.810	7,496	0.564	17	125	14	128	20	38 duplicate
14536	117 [724; Glycerol (3TMS)]	56 0.531	0.827	7,571	0.593	18	124	10	132	21	17 duplicate
17651	117 [724; Glycerol (3TMS)]	56 0.529	0.809	5,571	0.498	19	123	15	127	8	77 duplicate
18377	117 [724; Glycerol (3TMS)]	53 0.517	0.783	18,828	0.641	20	122	20	122	93	7 duplicate
13234	117 [724; Glycerol (3TMS)]	56 0.514	0.752	16,400	0.522	21	120	30	112	81	60 duplicate
19121	117 [724; Glycerol (3TMS)]	56 0.512	0.689	6,996	0.580	23	119	41	101	17	29 duplicate
19511	117 [724; Glycerol (3TMS)]	48 0.496	0.767	5,830	0.591	24	118	24	118	9	19 duplicate
19484	117 [724; Glycerol (3TMS)]	56 0.492	0.693	6,053	0.555	25	117	40	102	10	44 duplicate
16781	117 [724; Glycerol (3TMS)]	56 0.482	0.736	14,198	0.571	26	116	35	107	66	33 duplicate
12649	117 [724; Glycerol (3TMS)]	56 0.478	0.686	16,335	0.513	27	115	42	100	79	66 duplicate
17377	117 [724; Glycerol (3TMS)]	50 0.474	0.526	18,365	0.472	28	114	60	82	91	94 duplicate
13573	117 [724; Glycerol (3TMS)]	56 0.460	0.741	6,851	0.597	29	113	33	109	15	13 duplicate
16282	117 [724; Glycerol (3TMS)]	56 0.453	0.677	6,377	0.582	30	112	27	115	11	26 duplicate
18322	117 [724; Glycerol (3TMS)]	40 0.451	0.791	7,055	0.546	31	111	17	125	18	49 duplicate
9660	117 [724; Glycerol (3TMS)]	55 0.449	0.775	23,626	0.604	32	110	22	120	118	10 original
19196	117 [724; Glycerol (3TMS)]	55 0.448	0.682	6,687	0.529	33	109	45	97	14	57 duplicate
13003	117 [724; Glycerol (3TMS)]	56 0.445	0.775	30,971	0.597	34	108	21	121	129	14 duplicate
11533	117 [724; Glycerol (3TMS)]	55 0.441	0.741	8,287	0.553	35	107	34	108	25	45 duplicate
11404	117 [724; Glycerol (3TMS)]	56 0.438	0.682	8,610	0.535	36	106	44	98	29	53 duplicate
12039	117 [724; Glycerol (3TMS)]	56 0.434	0.755	17,289	0.596	37	105	29	113	87	15 duplicate
12408	117 [724; Glycerol (3TMS)]	56 0.432	0.684	11,249	0.521	38	104	43	99	48	62 duplicate

9661	117 [724; Glycerol (3TMS)]	56	0.426	0.625	12.927	0.515	39	103	49	93	55	65 original
11661	117 [724; Glycerol (3TMS)]	56	0.425	0.759	15.220	0.607	40	102	25	117	73	8 duplicate
9646	117 [724; Glycerol (3TMS)]	51	0.420	0.228	12.863	0.552	41	101	74	68	54	47 original
17012	117 [724; Glycerol (3TMS)]	56	0.419	0.787	7.781	0.588	42	100	19	123	23	24 duplicate
18484	117 [724; Glycerol (3TMS)]	58	0.417	0.662	11.031	0.581	43	99	47	95	45	28 duplicate
15694	117 [724; Glycerol (3TMS)]	54	0.414	0.723	14.413	0.552	44	98	37	105	68	48 duplicate
12286	117 [724; Glycerol (3TMS)]	56	0.414	0.615	8.568	0.494	45	97	51	91	28	79 duplicate
15324	117 [724; Glycerol (3TMS)]	56	0.412	0.755	15.001	0.592	46	96	28	114	71	18 duplicate
9655	117 [724; Glycerol (3TMS)]	55	0.410	0.746	8.007	0.561	47	95	32	110	24	40 original
14839	117 [724; Glycerol (3TMS)]	56	0.404	0.616	13.221	0.483	48	94	50	92	61	87 duplicate
9658	117 [724; Glycerol (3TMS)]	40	0.403	0.750	11.481	0.533	49	93	31	111	51	54 original
19456	117 [724; Glycerol (3TMS)]	56	0.397	0.610	13.876	0.492	50	92	52	90	65	83 duplicate
9651	117 [724; Glycerol (3TMS)]	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	0.590	31.102	0.504	51	91	54	88	130	73 original
19159	117 [724; Glycerol (3TMS)]	56	0.395	0.521	13.151	0.488	52	90	62	80	60	86 duplicate
10744	117 [724; Glycerol (3TMS)]	56	0.375	0.609	40.164	0.544	53	89	53	89	141	50 duplicate
9653	117 [724; Glycerol (3TMS)]	56	0.374	0.560	5.246	0.504	54	88	55	87	4	72 original
12163	117 [724; Glycerol (3TMS)]	39	0.374	0.704	17.210	0.562	55	87	39	103	86	38 duplicate
18686	117 [724; Glycerol (3TMS)]	50	0.365	0.525	7.471	0.513	56	86	61	81	19	68 duplicate
18376	117 [724; Glycerol (3TMS)]	51	0.358	0.708	10.799	0.569	57	85	38	104	44	35 duplicate
9649	117 [724; Glycerol (3TMS)]	56	0.356	0.528	11.331	0.540	58	84	59	83	50	52 original
9654	117 [724; Glycerol (3TMS)]	43	0.353	0.560	6.881	0.509	59	83	56	86	13	70 original
19366	117 [724; Glycerol (3TMS)]	56	0.313	0.735	19.956	0.527	60	82	36	106	102	58 duplicate
19232	117 [724; Glycerol (3TMS)]	46	0.304	0.482	10.615	0.504	61	81	65	77	42	74 duplicate
9666	117 [724; Glycerol (3TMS)]	42	0.296	0.441	13.481	0.381	62	80	67	76	62	129 original
19082	117 [724; Glycerol (3TMS)]	56	0.291	0.358	11.306	0.408	63	79	71	71	49	118 duplicate
18431	117 [724; Glycerol (3TMS)]	54	0.284	0.556	33.588	0.482	64	78	58	84	136	88 duplicate
18709	117 [724; Glycerol (3TMS)]	56	0.277	0.662	19.964	0.527	65	77	46	96	103	59 duplicate
18201	117 [724; Glycerol (3TMS)]	50	0.264	0.085	20.929	0.380	66	76	84	58	109	130 duplicate
9667	117 [724; Glycerol (3TMS)]	53	0.241	0.429	11.223	0.417	67	75	68	74	47	114 original
16048	117 [724; Glycerol (3TMS)]	49	0.226	0.559	8.406	0.502	68	74	57	85	26	76 duplicate
18916	117 [724; Glycerol (3TMS)]	49	0.218	0.334	20.186	0.493	69	73	72	70	104	82 duplicate
9664	117 [724; Glycerol (3TMS)]	41	0.217	0.408	14.441	0.437	70	72	69	73	69	106 original
18032	117 [724; Glycerol (3TMS)]	54	0.209	0.454	29.562	0.451	71	71	66	76	126	98 duplicate
19427	117 [724; Glycerol (3TMS)]	38	0.195	0.225	18.832	0.475	72	70	76	68	94	91 duplicate
18872	117 [724; Glycerol (3TMS)]	42	0.194	0.186	16.998	0.319	73	69	79	63	83	141 duplicate
9659	117 [724; Glycerol (3TMS)]	56	0.188	0.226	9.602	0.402	74	68	75	67	35	123 original
18637	117 [724; Glycerol (3TMS)]	56	0.187	0.203	17.688	0.437	75	67	78	64	89	105 duplicate
19562	117 [724; Glycerol (3TMS)]	26	0.175	0.493	7.679	0.505	76	66	64	78	22	71 duplicate
17971	117 [724; Glycerol (3TMS)]	56	0.155	0.401	34.165	0.497	77	65	70	72	137	78 duplicate
9663	117 [724; Glycerol (3TMS)]	56	0.122	0.135	14.774	0.394	78	64	81	61	70	126 original
9662	117 [724; Glycerol (3TMS)]	17	0.088	0.247	4.617	0.478	79	63	73	69	3	90 original
17447	117 [724; Glycerol (3TMS)]	56	0.087	0.211	13.023	0.474	80	62	77	65	57	82 duplicate
9644	117 [724; Glycerol (3TMS)]	54	0.085	0.171	9.895	0.372	81	61	80	62	36	135 original
19001	117 [724; Glycerol (3TMS)]	39	0.082	0.512	9.281	0.581	82	60	63	79	32	39 duplicate
9650	117 [724; Glycerol (3TMS)]	51	0.081	0.079	20.963	0.445	83	59	85	57	110	101 original
9645	117 [724; Glycerol (3TMS)]	56	0.073	0.116	9.861	0.410	84	58	82	60	37	117 original
9665	117 [724; Glycerol (3TMS)]	34	0.023	0.021	17.057	0.324	85	57	88	54	85	140 original

11914	117 [724; Glycerol (3TMS)]	15 Alanine	56 0,017	0,087	19,216	0,513	88	56	83	59	98	67 duplicate
15418	117 [724; Glycerol (3TMS)]	47 [NA]	56 0,004	-0,098	13,090	0,531	87	55	92	50	58	55 duplicate
18734	117 [724; Glycerol (3TMS)]	93 [607; Putrescine (4TMS)]	53 0,000	-0,047	15,156	0,371	88	54	86	56	72	137 duplicate
18936	117 [724; Glycerol (3TMS)]	84 [789; Tyramine (3TMS)]	55 -0,002	-0,024	8,563	0,383	89	53	89	53	27	128 duplicate
18266	117 [724; Glycerol (3TMS)]	84 Mannitol	54 -0,040	0,026	31,882	0,494	90	52	87	55	132	81 duplicate
14329	117 [724; Glycerol (3TMS)]	36 [596; N-Acetylglutamic acid (2TMS)]	56 -0,040	-0,119	27,868	0,418	91	51	93	49	121	113 duplicate
18587	117 [724; Glycerol (3TMS)]	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	56 -0,068	-0,056	9,982	0,332	92	50	90	52	38	139 duplicate
16459	117 [724; Glycerol (3TMS)]	[636; 4R-Acetylmido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	56 -0,077	-0,092	17,028	0,420	93	48	91	51	84	111 duplicate
19301	117 [724; Glycerol (3TMS)]	107 9-(Z)-Octadecenoic acid	56 -0,077	-0,136	15,311	0,373	94	49	95	47	74	133 duplicate
10473	117 [724; Glycerol (3TMS)]	4 Phosphoric acid	43 -0,083	-0,135	31,489	0,348	95	47	94	48	131	138 duplicate
9656	117 [724; Glycerol (3TMS)]	130 Trehalose	55 -0,108	-0,148	28,787	0,462	96	46	97	45	123	97 original
17117	117 [724; Glycerol (3TMS)]	75 Lysine	56 -0,109	-0,147	37,816	0,420	97	45	96	46	138	112 duplicate
17516	117 [724; Glycerol (3TMS)]	72 [919; D-Xylopyranose (4TMS)]	55 -0,127	-0,167	11,520	0,398	98	44	99	43	52	124 duplicate
17161	117 [724; Glycerol (3TMS)]	67 Citric acid	56 -0,151	-0,193	23,495	0,402	99	43	101	41	117	122 duplicate
16622	117 [724; Glycerol (3TMS)]	60 Glycerol-3-phosphate	56 -0,160	-0,181	21,395	0,433	100	41	98	44	113	108 duplicate
15961	117 [724; Glycerol (3TMS)]	53 Glycerol-2-phosphate	56 -0,213	-0,225	11,211	0,376	101	42	102	40	46	132 duplicate
10878	117 [724; Glycerol (3TMS)]	7 Threonine	56 -0,243	-0,347	10,029	0,520	103	39	107	35	39	124
18334	117 [724; Glycerol (3TMS)]	66 Glyceral acid-3-phosphate	56 -0,266	-0,352	10,757	0,440	104	38	108	34	43	104 duplicate
10336	117 [724; Glycerol (3TMS)]	3 Ethanolamine	54 -0,279	-0,463	13,577	0,511	105	37	112	30	63	69 duplicate
10198	117 [724; Glycerol (3TMS)]	2 Serine	54 -0,315	-0,313	21,045	0,408	106	36	106	36	111	119 duplicate
15873	117 [724; Glycerol (3TMS)]	52 [NA]	39 -0,317	-0,563	19,446	0,544	107	35	117	25	98	51 duplicate
14433	117 [724; Glycerol (3TMS)]	37 Phenylalanine	56 -0,323	-0,397	22,809	0,406	108	34	109	33	115	120 duplicate
11143	117 [724; Glycerol (3TMS)]	9 Proline	55 -0,325	-0,305	28,043	0,379	109	33	105	37	122	131 duplicate
13764	117 [724; Glycerol (3TMS)]	31 [622; Parabanic acid (2TMS)]	56 -0,339	-0,525	12,943	0,490	110	32	114	28	56	84 duplicate
10059	117 [724; Glycerol (3TMS)]	1 [938; Sulfuric acid (2TMS)]	35 -0,358	-0,189	10,583	0,581	111	31	100	42	41	27 duplicate
16541	117 [724; Glycerol (3TMS)]	59 Ornithine; Arginine	56 -0,360	-0,419	39,223	0,423	112	30	110	32	139	110 duplicate
13348	117 [724; Glycerol (3TMS)]	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	45 -0,372	-0,743	21,191	0,494	113	29	130	12	112	80 duplicate
18092	117 [724; Glycerol (3TMS)]	81 Tyrosine	56 -0,383	-0,507	32,844	0,591	114	28	113	29	134	20 duplicate
17846	117 [724; Glycerol (3TMS)]	[826; beta-[[[5-methyl-2-thienyl)methyl]amino-77 benzeneacetic acid methyl ester]	54 -0,384	-0,457	29,473	0,405	115	27	111	31	125	121 duplicate
11011	117 [724; Glycerol (3TMS)]	8 Isoleucine	47 -0,393	-0,278	20,516	0,372	116	26	104	38	106	134 duplicate
18827	117 [724; Glycerol (3TMS)]	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	42 -0,403	-0,604	16,224	0,434	117	25	120	22	77	107 duplicate
15036	117 [724; Glycerol (3TMS)]	43 [548; Leucine (2TBS)]	52 -0,410	-0,584	12,258	0,397	118	24	119	23	63	125 duplicate
12866	117 [724; Glycerol (3TMS)]	23 Homoserine	56 -0,429	-0,764	16,279	0,522	119	23	132	10	78	61 duplicate
15511	117 [724; Glycerol (3TMS)]	48 Asparagine	56 -0,436	-0,704	16,456	0,516	120	22	126	16	82	64 duplicate
11274	117 [724; Glycerol (3TMS)]	10 Glycine	56 -0,439	-0,767	20,763	0,587	121	21	133	9	107	21 duplicate
18859	117 [724; Glycerol (3TMS)]	63 Glutamine	46 -0,443	-0,620	19,157	0,556	122	20	123	19	95	42 duplicate
13903	117 [724; Glycerol (3TMS)]	32 [729; N,N-Dimethyllysine methyl ester]	55 -0,444	-0,812	19,885	0,530	123	19	121	21	100	56 duplicate
16702	117 [724; Glycerol (3TMS)]	61 [NA]	56 -0,482	-0,615	10,518	0,442	124	18	122	20	40	103 duplicate
14118	117 [724; Glycerol (3TMS)]	34 Aspartic acid	56 -0,490	-0,550	32,452	0,411	125	17	116	26	133	115 duplicate
13684	117 [724; Glycerol (3TMS)]	30 [915; Ethyl-3-(2H)-thiophenone]	56 -0,508	-0,547	30,009	0,372	126	16	115	27	127	136 duplicate
14011	117 [724; Glycerol (3TMS)]	33 Methionine	56 -0,517	-0,640	15,958	0,424	127	15	125	17	76	109 duplicate
17306	117 [724; Glycerol (3TMS)]	69 Arginine	52 -0,517	-0,748	23,389	0,555	128	14	131	11	116	43 duplicate
16134	117 [724; Glycerol (3TMS)]	42 Glutamic acid	52 -0,525	-0,574	30,205	0,385	129	13	118	24	128	127 duplicate
15784	117 [724; Glycerol (3TMS)]	55 [912; 4-Aminobutyric acid (2TBS)]	35 -0,529	-0,624	20,260	0,470	130	12	124	18	105	95 duplicate
15229	117 [724; Glycerol (3TMS)]	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	37 -0,535	-0,732	17,429	0,479	131	11	129	13	88	89 duplicate
18959	117 [724; Glycerol (3TMS)]	49 Homocysteine	53 -0,546	-0,731	19,798	0,445	132	10	128	14	99	100 duplicate
13119	117 [724; Glycerol (3TMS)]	98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	42 -0,554	-0,846	17,955	0,573	133	9	138	4	90	31 duplicate
		25 [709; 2,5-Diaminovalerolactam (2TMS)]	45 -0,564	-0,790	19,284	0,557	134	8	135	7	97	41 duplicate

17234	117 [724; Glycerol (3TMS)]	68 [570; Hypoxanthine (2TMS)]	16 -0.583	-0.895	13,100	0.451	135	7	141	1	59	99 duplicate
15603	117 [724; Glycerol (3TMS)]	49 [877; Pyrophosphoric acid (4TMS)]	56 -0.587	-0.705	22,324	0.470	136	6	127	15	114	96 duplicate
9657	117 [724; Glycerol (3TMS)]	131 [626; 5-Methylthioadenosine (3TMS)]	49 -0.595	-0.787	16,395	0.503	137	5	134	8	80	75 original
18536	117 [724; Glycerol (3TMS)]	89 [775; Dopamine (4TMS)]	28 -0.614	-0.814	18,670	0.488	138	4	137	5	92	85 duplicate
12529	117 [724; Glycerol (3TMS)]	20 [618; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	23 -0.621	-0.804	14,350	0.572	139	3	136	6	67	32 duplicate
18151	117 [724; Glycerol (3TMS)]	82 Lysine	32 -0.649	-0.894	19,952	0.604	140	2	140	2	101	11 duplicate
10609	117 [724; Glycerol (3TMS)]	5 Leucine	38 -0.653	-0.884	15,620	0.549	141	1	139	3	75	48 duplicate
18033	118 [928; Glucopyranose-6- $\beta$ ]	80 [772; D-Glucose (5TMS)]	56 0.604	0.799	29,950	0.500	1	141	1	141	125	3 duplicate
17517	118 [928; Glucopyranose-6- $\beta$ ]	72 [918; D-Xylopyranose (4TMS)]	57 0.474	0.567	6,687	0.409	2	140	4	138	3	61 duplicate
14840	118 [928; Glucopyranose-6- $\beta$ ]	41 [639; Proline (2TMS)]	58 0.407	0.613	14,416	0.420	3	139	3	139	67	53 duplicate
18432	118 [928; Glucopyranose-6- $\beta$ ]	87 [945; beta-D-Glucopyranose (5TMS)]	56 0.379	0.696	34,978	0.493	4	138	2	140	135	5 duplicate
15419	118 [928; Glucopyranose-6- $\beta$ ]	47 [NA]	58 0.304	0.501	9,573	0.457	5	137	6	136	18	17 duplicate
12409	118 [928; Glucopyranose-6- $\beta$ ]	19 Alanine (BP) (3TMS)	58 0.289	0.554	12,784	0.434	6	136	5	137	53	43 duplicate
9672	118 [928; Glucopyranose-6- $\beta$ ]	123 [945; Galactofuranose-6-phosphate (7TMS)]	58 0.275	0.430	12,303	0.409	7	135	9	133	49	62 original
9688	118 [928; Glucopyranose-6- $\beta$ ]	139 [700; Ergosta-5,7-dien-3-ol]	33 0.254	0.172	13,078	0.476	8	134	34	108	55	8 original
11915	118 [928; Glucopyranose-6- $\beta$ ]	15 Alanine	58 0.239	0.467	19,429	0.423	9	133	7	135	99	50 duplicate
19512	118 [928; Glucopyranose-6- $\beta$ ]	114 Fructose-6-phosphate	51 0.227	0.347	7,506	0.464	10	132	13	129	5	14 duplicate
17972	118 [928; Glucopyranose-6- $\beta$ ]	79 Glucose	58 0.205	0.407	35,731	0.426	11	131	10	132	137	47 duplicate
16460	118 [928; Glucopyranose-6- $\beta$ ]	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	58 0.176	0.109	17,327	0.309	12	130	48	94	84	134 duplicate
18873	118 [928; Glucopyranose-6- $\beta$ ]	96 myo-Inositol	43 0.169	0.070	14,372	0.307	13	129	62	80	65	135 duplicate
19485	118 [928; Glucopyranose-6- $\beta$ ]	113 Galactose-6-phosphate	58 0.165	0.378	7,723	0.441	14	128	12	130	6	30 duplicate
19563	118 [928; Glucopyranose-6- $\beta$ ]	116 [882; Pseudouridine (5TMS)]	29 0.158	-0.154	10,419	0.358	15	127	98	44	24	102 duplicate
10474	118 [928; Glucopyranose-6- $\beta$ ]	4 Phosphoric acid	45 0.156	0.134	32,329	0.311	16	126	43	99	129	132 duplicate
17378	118 [928; Glucopyranose-6- $\beta$ ]	70 [893; 2-Furan-2-hydroxyacetic acid (2TMS)]	51 0.153	0.283	19,710	0.413	17	125	18	124	100	57 duplicate
19167	118 [928; Glucopyranose-6- $\beta$ ]	104 [785; Erythritol (4TMS)]	57 0.145	0.235	9,334	0.396	18	124	25	117	15	72 duplicate
9687	118 [928; Glucopyranose-6- $\beta$ ]	138 [674; Ergosterol (1TMS)]	42 0.145	0.207	11,793	0.406	19	123	31	111	44	68 original
9885	118 [928; Glucopyranose-6- $\beta$ ]	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17 0.118	0.221	3,803	0.319	20	122	28	114	1	124 original
9670	118 [928; Glucopyranose-6- $\beta$ ]	121 [657; Erythritol (4TMS)]	51 0.111	0.247	10,507	0.440	21	121	22	120	29	33 original
19063	118 [928; Glucopyranose-6- $\beta$ ]	101 [832; Dopamine (4TMS)]	58 0.107	0.163	12,754	0.379	22	120	38	104	52	85 duplicate
13235	118 [928; Glucopyranose-6- $\beta$ ]	26 Citramalic acid	58 0.103	0.180	17,968	0.346	23	119	33	109	87	111 duplicate
9689	118 [928; Glucopyranose-6- $\beta$ ]	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	43 0.103	0.011	11,479	0.463	24	118	71	71	39	18 original
16937	118 [928; Glucopyranose-6- $\beta$ ]	64 [789; Tyramine (3TMS)]	58 0.100	0.049	7,903	0.380	25	117	58	84	7	82 duplicate
17718	118 [928; Glucopyranose-6- $\beta$ ]	75 Lysine	58 0.081	0.077	10,154	0.357	26	116	67	75	22	104 original
19587	118 [928; Glucopyranose-6- $\beta$ ]	117 [724; Glycerol (3TMS)]	58 0.080	0.068	39,511	0.312	27	115	64	78	138	130 duplicate
19538	118 [928; Glucopyranose-6- $\beta$ ]	115 Glucose-6-phosphate	54 0.085	0.171	9,895	0.372	28	114	35	107	19	93 duplicate
12769	118 [928; Glucopyranose-6- $\beta$ ]	22 [690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	58 0.082	0.319	26,407	0.525	29	113	17	125	118	1 duplicate
18210	118 [928; Glucopyranose-6- $\beta$ ]	83 Sorbitol	51 0.078	0.105	10,629	0.360	30	112	50	92	32	101 duplicate
19268	118 [928; Glucopyranose-6- $\beta$ ]	108 [733; Threitol (4TMS)]	52 0.072	0.093	21,747	0.298	31	111	56	88	109	137 duplicate
19398	118 [928; Glucopyranose-6- $\beta$ ]	110 [715; Erythritol (4TMS)]	57 0.071	0.240	12,721	0.399	32	110	24	118	51	70 duplicate
14225	118 [928; Glucopyranose-6- $\beta$ ]	35 Pyrogulamic acid	52 0.057	0.267	11,288	0.446	33	109	20	122	38	26 duplicate
9674	118 [928; Glucopyranose-6- $\beta$ ]	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	58 0.055	0.338	41,989	0.475	34	108	14	128	140	9 duplicate
12287	118 [928; Glucopyranose-6- $\beta$ ]	18 [590; 1-Acetyl-2-thiohydantoin]	58 0.051	0.446	33,005	0.440	35	107	8	134	130	35 original
9679	118 [928; Glucopyranose-6- $\beta$ ]	130 Trehalose	58 0.049	0.102	10,356	0.351	36	106	52	90	23	108 duplicate
9681	118 [928; Glucopyranose-6- $\beta$ ]	132 [895; Isomaltose methoxamine (8TMS)]	41 0.048	-0.075	30,590	0.364	37	105	59	83	127	100 original
14330	118 [928; Glucopyranose-6- $\beta$ ]	36 [596; N-Acetylglutamic acid (2TMS)]	58 0.041	-0.078	14,315	0.436	38	104	85	57	63	40 original
17585	118 [928; Glucopyranose-6- $\beta$ ]	73 [708; Glucose methoxamine (5TMS)]	51 0.038	-0.009	29,279	0.318	39	103	72	70	122	125 duplicate
19160	118 [928; Glucopyranose-6- $\beta$ ]	103 [648; Ethylamine (2TMS)]	58 0.034	0.170	10,473	0.365	40	102	36	106	28	97 duplicate
16782	118 [928; Glucopyranose-6- $\beta$ ]	62 [812; D-Xylofuranose (4TMS)]	58 0.022	0.102	16,515	0.357	41	101	51	91	80	105 duplicate
				0.198	16,045	0.463	42	99	32	110	77	15 duplicate

11789	118 [928; Glucopyranose-6-]	14	Fumaric acid	58	0.022	0.117	8.153	0.375	43	100	47	95	9	89 duplicate
17652	118 [928; Glucopyranose-6-]	74	[912; Tetradecanoic acid (1TMS)]	58	0.020	0.119	11.505	0.373	44	98	46	96	40	92 duplicate
13462	118 [928; Glucopyranose-6-]	28	Malic acid	58	0.019	0.089	11.778	0.406	45	97	57	85	43	65 duplicate
10199	118 [928; Glucopyranose-6-]	2	Serine	56	0.018	0.012	19.989	0.336	46	96	70	72	104	114 duplicate
13349	118 [928; Glucopyranose-6-]	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	47	0.018	-0.138	18.114	0.310	47	95	95	47	90	133 duplicate
10745	118 [928; Glucopyranose-6-]	6	Glycerol	58	0.018	0.384	42.217	0.434	48	94	11	131	141	42 duplicate
12650	118 [928; Glucopyranose-6-]	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	58	0.008	0.068	18.541	0.372	49	93	63	78	93	94 duplicate
18638	118 [928; Glucopyranose-6-]	91	[766; beta-D-Methylglucopyranoside (4TMS)]	58	0.004	0.057	19.122	0.352	50	92	68	76	97	107 duplicate
17810	118 [928; Glucopyranose-6-]	78	Mannose	56	0.003	0.227	10.637	0.421	51	91	28	116	33	52 duplicate
12164	118 [928; Glucopyranose-6-]	17	[700; 2-methyl-1,2-propanediol (2TMS)]	46	-0.001	0.134	13.610	0.436	52	90	40	102	102	29 duplicate
13120	118 [928; Glucopyranose-6-]	25	[709; 2,5-Diaminovalerolactam (2TMS)]	58	-0.001	0.150	19.850	0.443	53	89	44	98	59	39 duplicate
13904	118 [928; Glucopyranose-6-]	32	[728; N,N-Dimethyllysine methyl ester]	57	-0.006	-0.082	15.834	0.350	54	88	81	61	75	109 duplicate
15037	118 [928; Glucopyranose-6-]	43	[548; Leucine (2TBS)]	54	-0.008	-0.071	10.426	0.325	55	87	84	58	25	120 duplicate
18323	118 [928; Glucopyranose-6-]	85	[529; Methylcitric acid (4TMS)]	42	-0.010	0.060	7.467	0.381	56	86	65	77	4	81 duplicate
11405	118 [928; Glucopyranose-6-]	11	Succinic acid	58	-0.011	0.107	10.465	0.437	57	85	49	93	27	37 duplicate
17783	118 [928; Glucopyranose-6-]	78	Fructose	58	-0.014	0.338	27.071	0.449	58	84	15	127	119	24 duplicate
17013	118 [928; Glucopyranose-6-]	65	[646; 3-Deoxyglucitol (5TMS)]	58	-0.015	0.218	13.687	0.517	59	83	29	113	60	2 duplicate
11662	118 [928; Glucopyranose-6-]	13	Uracil	55	-0.020	0.156	18.544	0.431	60	82	39	103	94	46 duplicate
16293	118 [928; Glucopyranose-6-]	141	Lanosta-8,24-dien-3-beta-ol	55	-0.021	-0.159	12.164	0.425	61	81	100	42	47	48 original
9690	118 [928; Glucopyranose-6-]	56	[829; Orotic acid (3TMS)]	58	-0.021	0.241	11.097	0.467	62	80	23	119	37	11 duplicate
16293	118 [928; Glucopyranose-6-]	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	39	-0.023	0.072	6.652	0.411	63	79	81	81	2	58 original
15695	118 [928; Glucopyranose-6-]	50	[746; Ribonic acid-1,4-lactone (3TMS)]	57	-0.024	0.167	14.846	0.410	64	78	37	105	71	60 duplicate
14537	118 [928; Glucopyranose-6-]	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	58	-0.028	0.094	10.590	0.399	65	77	55	87	31	69 duplicate
14740	118 [928; Glucopyranose-6-]	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	58	-0.033	0.017	35.246	0.371	66	76	69	73	136	96 duplicate
9678	118 [928; Glucopyranose-6-]	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	57	-0.034	0.211	13.137	0.445	67	75	30	112	57	27 original
9669	118 [928; Glucopyranose-6-]	120	[945; Uridine (3TMS)]	53	-0.035	-0.070	14.325	0.388	68	74	83	59	64	78 original
17088	118 [928; Glucopyranose-6-]	66	Glycic acid-3-phosphate	58	-0.038	-0.091	8.447	0.336	69	73	87	55	11	115 duplicate
18465	118 [928; Glucopyranose-6-]	88	Gluconic acid	58	-0.039	0.140	14.555	0.457	70	72	42	100	68	18 duplicate
15325	118 [928; Glucopyranose-6-]	46	Arabinose	58	-0.041	0.251	19.139	0.454	71	71	21	121	88	20 duplicate
17448	118 [928; Glucopyranose-6-]	71	[731; Erythrose (3TMS)]	58	-0.042	-0.119	14.243	0.331	72	70	91	51	62	118 duplicate
12040	118 [928; Glucopyranose-6-]	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	58	-0.044	0.095	20.025	0.441	73	69	54	88	105	32 duplicate
11144	118 [928; Glucopyranose-6-]	9	Proline	57	-0.045	-0.020	28.154	0.324	74	68	74	68	121	121 duplicate
19043	118 [928; Glucopyranose-6-]	100	[857; Mannitol (6TMS)]	58	-0.051	-0.215	12.030	0.455	75	67	110	32	46	19 duplicate
9683	118 [928; Glucopyranose-6-]	134	Isomaltose	58	-0.053	0.226	27.081	0.440	76	65	27	115	120	34 original
14639	118 [928; Glucopyranose-6-]	39	Glycerol-3-phosphate	58	-0.053	-0.183	22.801	0.375	77	66	104	38	112	90 duplicate
18378	118 [928; Glucopyranose-6-]	122	[644; Erythritol (4TMS)]	58	-0.060	0.098	18.937	0.400	78	64	53	89	85	68 duplicate
9671	118 [928; Glucopyranose-6-]	86	[793; 1-Phenylethanol (1TMS)]	49	-0.061	-0.047	13.874	0.425	79	63	78	64	61	49 original
13004	118 [928; Glucopyranose-6-]	24	[725; 2-Ketooctanoic acid (2TMS)]	55	-0.064	0.148	33.621	0.445	80	62	19	123	113	25 duplicate
18782	118 [928; Glucopyranose-6-]	94	Hexadecanoic acid	58	-0.064	0.030	23.057	0.414	82	61	68	74	114	28 duplicate
19367	118 [928; Glucopyranose-6-]	109	Octadecanoic acid	58	-0.065	0.074	24.087	0.408	83	59	60	82	116	56 duplicate
18687	118 [928; Glucopyranose-6-]	92	[680; Glycerol-2-phosphate (4TMS)]	50	-0.081	0.327	7.977	0.495	84	58	16	128	8	4 duplicate
10879	118 [928; Glucopyranose-6-]	7	Threonine	58	-0.088	-0.106	30.948	0.317	85	56	90	52	128	127 duplicate
9686	118 [928; Glucopyranose-6-]	137	Ergosterol	58	-0.088	-0.257	16.874	0.336	86	57	114	28	81	116 original
17947	118 [928; Glucopyranose-6-]	77	[826; beta-[[5-methyl-2-thienyl)methyl]phenylamino-benzeneacetic acid methyl ester]	56	-0.088	-0.191	29.874	0.335	87	55	107	35	124	117 duplicate
18093	118 [928; Glucopyranose-6-]	81	Tyrosine	58	-0.089	-0.279	34.197	0.438	88	54	116	26	134	36 duplicate
17307	118 [928; Glucopyranose-6-]	69	Arginine	54	-0.094	-0.164	22.279	0.354	90	52	101	41	110	106 duplicate
9673	118 [928; Glucopyranose-6-]	124	[734; 1-Monocleoylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	53	-0.097	-0.134	19.771	0.417	91	51	94	48	101	55 original



19457	118 [928; Glucopyranose-6-]	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	58 -0,099	-0,099	13,102	0,450	92	50	88	54	58	23-juplicate
14119	118 [928; Glucopyranose-6-]	34 Aspartic acid	58 -0,101	-0,080	33,289	0,321	93	49	86	58	131	123-juplicate
16542	118 [928; Glucopyranose-6-]	59 Ornithine; Arginine	58 -0,103	-0,128	40,848	0,329	94	48	92	50	139	118-juplicate
15230	118 [928; Glucopyranose-6-]	45 Homocysteine	55 -0,104	-0,170	18,021	0,317	95	47	102	40	88	128-juplicate
19428	118 [928; Glucopyranose-6-]	111 [583; Erythritol (4TMS)]	40 -0,105	-0,282	16,505	0,382	96	46	117	25	79	80-juplicate
14012	118 [928; Glucopyranose-6-]	33 Methionine	58 -0,108	-0,066	12,917	0,315	97	45	82	60	54	129-juplicate
9884	118 [928; Glucopyranose-6-]	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	58 -0,113	-0,148	14,377	0,394	98	44	96	46	66	73 original
18917	118 [928; Glucopyranose-6-]	97 [756; beta-D-Methylglucopyranoside (4TMS)]	50 -0,118	-0,041	22,488	0,441	99	43	76	68	111	31-juplicate
13574	118 [928; Glucopyranose-6-]	29 Erythritol	58 -0,122	-0,012	8,445	0,391	100	42	73	69	10	75-juplicate
16377	118 [928; Glucopyranose-6-]	57 [757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	54 -0,126	0,127	15,873	0,432	101	41	45	97	76	44-juplicate
9675	118 [928; Glucopyranose-6-]	126 [559; Erythritol (4TMS)]	45 -0,127	-0,155	9,465	0,422	102	40	99	43	16	51 original
13685	118 [928; Glucopyranose-6-]	30 [815; Ethyl-3-(2H)-thiophenone]	58 -0,129	-0,081	30,243	0,322	103	39	80	62	126	122-juplicate
14939	118 [928; Glucopyranose-6-]	42 Glutamic acid	54 -0,129	-0,130	29,604	0,341	104	38	93	49	123	112-juplicate
13795	118 [928; Glucopyranose-6-]	31 [622; Parabanic acid (2TMS)]	58 -0,131	-0,191	10,507	0,312	105	36	106	36	30	131-juplicate
15804	118 [928; Glucopyranose-6-]	49 [877; Pyrophosphoric acid (4TMS)]	58 -0,131	-0,285	18,965	0,378	106	37	118	24	96	88-juplicate
11534	118 [928; Glucopyranose-6-]	12 Glyceric acid	57 -0,134	-0,106	9,489	0,411	107	35	89	53	17	59-juplicate
18960	118 [928; Glucopyranose-6-]	98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	42 -0,141	-0,223	16,880	0,284	108	34	112	30	82	138-juplicate
19335	118 [928; Glucopyranose-6-]	108 Octadecenoic acid	58 -0,146	-0,210	9,244	0,339	109	33	109	33	14	113-juplicate
12887	118 [928; Glucopyranose-6-]	23 Homoserine	58 -0,149	-0,190	13,373	0,372	110	32	105	37	58	95-juplicate
19122	118 [928; Glucopyranose-6-]	102 [904; Galactose methoxyamine (5TMS)]	58 -0,157	-0,309	8,753	0,452	111	31	120	22	13	22-juplicate
14434	118 [928; Glucopyranose-6-]	37 Phenylalanine	58 -0,162	-0,265	24,060	0,390	112	30	115	27	115	76-juplicate
17162	118 [928; Glucopyranose-6-]	67 Citric acid	58 -0,175	-0,323	25,004	0,349	113	28	121	21	117	110-juplicate
10060	118 [928; Glucopyranose-6-]	1 [938; Sulfuric acid (2TMS)]	34 -0,178	-0,209	8,478	0,435	114	28	108	34	12	41-juplicate
18828	118 [928; Glucopyranose-6-]	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	48 -0,178	-0,326	17,112	0,365	115	27	122	20	83	98-juplicate
11275	118 [928; Glucopyranose-6-]	10 Glycine	58 -0,180	-0,355	20,628	0,409	116	26	125	17	108	63-juplicate
16049	118 [928; Glucopyranose-6-]	54 [NA]	51 -0,183	-0,176	11,728	0,453	117	25	103	39	41	21-juplicate
16135	118 [928; Glucopyranose-6-]	55 [612; 4-Aminobutyric acid (2TBS)]	37 -0,189	-0,554	20,355	0,358	118	24	137	5	107	103-juplicate
15134	118 [928; Glucopyranose-6-]	44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	48 -0,190	-0,333	12,577	0,469	119	23	124	18	50	10-juplicate
11012	118 [928; Glucopyranose-6-]	8 Isoleucine	49 -0,190	-0,054	19,946	0,276	120	22	79	63	103	139-juplicate
15862	118 [928; Glucopyranose-6-]	53 Glyceral-2-phosphate	58 -0,192	-0,285	9,903	0,393	121	21	119	23	20	74-juplicate
18267	118 [928; Glucopyranose-6-]	84 Mannitol	56 -0,196	-0,151	33,320	0,379	122	20	97	45	132	83-juplicate
10337	118 [928; Glucopyranose-6-]	3 Ethanolamine	56 -0,205	-0,427	12,286	0,389	123	19	127	15	48	77-juplicate
9668	118 [928; Glucopyranose-6-]	119 [931; myo-Inositol-2-phosphate (7TMS)]	58 -0,211	-0,392	11,771	0,397	124	18	126	16	42	71 original
9677	118 [928; Glucopyranose-6-]	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	44 -0,211	-0,429	10,685	0,488	125	17	130	12	35	6 original
19233	118 [928; Glucopyranose-6-]	105 [705; 2-Ketogluconic acid (5TMS)]	47 -0,214	-0,332	14,799	0,432	126	16	123	19	70	45-juplicate
18152	118 [928; Glucopyranose-6-]	82 Lysine	33 -0,242	-0,456	18,210	0,404	127	15	134	8	91	67-juplicate
18735	118 [928; Glucopyranose-6-]	93 [607; Putrescine (4TMS)]	55 -0,262	-0,223	14,786	0,365	128	14	111	31	69	99-juplicate
19002	118 [928; Glucopyranose-6-]	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	40 -0,264	-0,045	10,438	0,488	129	13	77	65	28	7-juplicate
15512	118 [928; Glucopyranose-6-]	48 Asparagine	58 -0,266	-0,428	14,917	0,465	130	12	128	14	72	12-juplicate
19302	118 [928; Glucopyranose-6-]	107 9-(Z)-Octadecenoic acid	58 -0,267	-0,442	16,449	0,387	131	11	133	9	78	79-juplicate
9680	118 [928; Glucopyranose-6-]	131 [626; 5-Methylthioadenosine (3TMS)]	49 -0,282	-0,433	15,071	0,437	132	10	132	10	74	38 original
18588	118 [928; Glucopyranose-6-]	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	58 -0,297	-0,432	10,845	0,374	133	9	131	11	36	91-juplicate
10610	118 [928; Glucopyranose-6-]	5 Leucine	39 -0,323	-0,245	11,836	0,273	134	8	113	29	45	140-juplicate
16703	118 [928; Glucopyranose-6-]	61 [NA]	58 -0,325	-0,623	10,127	0,465	135	7	141	1	21	13-juplicate
12530	118 [928; Glucopyranose-6-]	20 [618; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	25 -0,333	-0,577	14,991	0,378	136	6	139	3	73	86-juplicate
15874	118 [928; Glucopyranose-6-]	52 [NA]	41 -0,334	-0,519	18,307	0,378	137	5	136	6	92	87-juplicate
16860	118 [928; Glucopyranose-6-]	53 Glutamine	47 -0,365	-0,564	17,608	0,418	138	4	138	4	85	54-juplicate
15785	118 [928; Glucopyranose-6-]	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	39 -0,387	-0,429	18,110	0,317	139	3	129	13	89	128-juplicate

17235	118 [928; Glucopyranose-6-]	68	[570; Hypoxanthine (2TMS)]	17	-0.441	-0.509	10.641	0.271	140	2	135	7	34	141 duplicate
18537	118 [928; Glucopyranose-6-]	89	[775; Dopamine (4TMS)]	30	-0.444	-0.610	17.859	0.298	141	1	140	2	86	138 duplicate
9712	119 [931; myo-Inositol-2-pho 141		Lanosta-8,24-dien-3-beta-ol	61	0.584	0.792	13.565	0.514	1	141	1	141	60	17 original
9708	119 [931; myo-Inositol-2-pho 137		Ergosterol	64	0.582	0.683	9.434	0.474	2	140	6	136	24	37 original
19303	119 [931; myo-Inositol-2-pho 107		9-(Z)-Octadecenoic acid	64	0.563	0.789	10.228	0.475	3	139	2	140	28	36 duplicate
18589	119 [931; myo-Inositol-2-pho 90		9-(Z)-Hexadecenoic acid (1TMS)]	64	0.498	0.643	4.446	0.514	4	138	5	137	2	15 duplicate
9697	119 [931; myo-Inositol-2-pho 128		[558; Erythritol (4TMS)]	45	0.489	0.644	6.167	0.511	5	137	9	133	5	19 original
9710	119 [931; myo-Inositol-2-pho 139		[700; Ergosta-5,7-dien-3-ol]	38	0.454	0.725	20.015	0.515	6	136	3	139	106	14 original
12531	119 [931; myo-Inositol-2-pho													
	20	[619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	31	0.441	0.556	14.956	0.608	7	135	14	128	69	1	1 duplicate
	124	[734; 1-Monooleoylglycerol (2TMS); 1-Monoheptadecyloxyglycerol (1TMS)]												
9695	118 [931; myo-Inositol-2-pho		Monohexadecenoic acid	59	0.425	0.565	24.483	0.441	8	134	13	128	119	62 original
18783	119 [931; myo-Inositol-2-pho 94		Hexadecanoic acid	84	0.420	0.494	17.612	0.538	9	133	17	125	90	5 duplicate
9711	119 [931; myo-Inositol-2-pho 140		[692; Ergosta-7,22-dien-3-ol (1TMS)]	49	0.415	0.650	17.272	0.496	10	132	8	134	87	26 original
9703	119 [931; myo-Inositol-2-pho 132		[895; Isomaltose methoxyamine (8TMS)]	42	0.412	0.399	14.948	0.459	11	131	26	116	68	46 original
15875	119 [931; myo-Inositol-2-pho 52		[NA]	46	0.405	0.675	18.621	0.472	12	130	7	135	96	38 duplicate
9707	119 [931; myo-Inositol-2-pho 136		[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.397	0.483	3.026	0.369	13	129	19	123	1	118 original
18368	119 [931; myo-Inositol-2-pho 109		Octadecanoic acid	64	0.387	0.364	18.961	0.458	14	128	29	113	99	44 duplicate
17163	119 [931; myo-Inositol-2-pho 67		Citric acid	64	0.361	0.384	20.257	0.463	15	127	27	115	108	44 duplicate
19336	119 [931; myo-Inositol-2-pho 108		Octadecenoic acid	64	0.360	0.494	7.507	0.396	16	126	16	126	10	96 duplicate
19429	119 [931; myo-Inositol-2-pho 111		[583; Erythritol (4TMS)]	42	0.336	0.366	18.605	0.439	17	125	28	114	104	64 duplicate
9699	119 [931; myo-Inositol-2-pho 128		[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.333	0.339	7.628	0.434	18	124	32	110	12	70 original
18829	119 [931; myo-Inositol-2-pho 95		[770; 3,4,6-Tris(hydroxyphenyl)ethanolamine (5TMS)]	50	0.332	0.479	18.951	0.437	19	122	20	122	88	66 duplicate
15135	119 [931; myo-Inositol-2-pho 44		[910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	0.332	0.325	9.538	0.442	20	123	33	109	25	61 duplicate
9709	119 [931; myo-Inositol-2-pho 138		[874; Ergosterol (1TMS)]	46	0.329	0.490	17.662	0.481	21	121	18	124	91	32 original
16136	119 [931; myo-Inositol-2-pho 55		[612; 4-Aminobutyric acid (2TBS)]	43	0.318	0.490	21.142	0.488	22	120	10	132	113	29 duplicate
18153	119 [931; myo-Inositol-2-pho 82		Lysine	39	0.317	0.351	13.101	0.517	23	119	30	112	57	12 duplicate
19234	119 [931; myo-Inositol-2-pho 105		[705; 2-Ketogluconic acid (5TMS)]	48	0.298	0.473	10.777	0.439	24	118	21	121	33	63 duplicate
16861	119 [931; myo-Inositol-2-pho 63		Glutamine	52	0.282	0.599	14.322	0.463	25	116	12	130	65	43 duplicate
9693	119 [931; myo-Inositol-2-pho 122		[644; Erythritol (4TMS)]	52	0.282	0.411	14.499	0.455	26	117	24	118	66	51 original
16624	119 [931; myo-Inositol-2-pho 60		Glycerol-3-phosphate	62	0.270	0.423	17.712	0.444	27	115	23	119	93	59 duplicate
18538	119 [931; myo-Inositol-2-pho 89		[775; Dopamine (4TMS)]	35	0.267	0.536	15.992	0.452	28	114	15	127	77	54 duplicate
9698	119 [931; myo-Inositol-2-pho 127		[777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.255	0.448	4.766	0.471	29	113	22	120	3	40 original
17236	119 [931; myo-Inositol-2-pho 68		[570; Hypoxanthine (2TMS)]	20	0.242	0.630	16.372	0.478	30	112	11	131	80	35 duplicate
10338	119 [931; myo-Inositol-2-pho 3		Ethanolamine	62	0.234	0.400	11.222	0.435	31	111	25	117	37	69 duplicate
14940	119 [931; myo-Inositol-2-pho 42		Glutamic acid	60	0.217	0.169	26.802	0.401	32	110	47	95	124	91 duplicate
18564	119 [931; myo-Inositol-2-pho 116		[882; Pseudouridine (5TMS)]	30	0.209	0.698	8.334	0.438	33	109	4	138	18	65 duplicate
17653	119 [931; myo-Inositol-2-pho 74		[912; Tetradecanoic acid (1TMS)]	64	0.207	0.307	10.580	0.445	34	108	36	106	30	57 duplicate
18736	119 [931; myo-Inositol-2-pho 93		[607; Putrescine (4TMS)]	60	0.202	0.194	17.283	0.352	35	107	45	97	88	128 duplicate
	119 [931; myo-Inositol-2-pho		[826; beta-[[[5-methyl-2-thienyl)methyl]eneamino- benzeneacetic acid methyl ester]											
17948	119 [931; myo-Inositol-2-pho 37		Phenylalanine	62	0.201	0.221	28.496	0.377	36	106	42	100	123	113 duplicate
14435	119 [931; myo-Inositol-2-pho 37		Phenylalanine	64	0.199	0.269	19.266	0.405	37	105	40	102	102	87 duplicate
18268	119 [931; myo-Inositol-2-pho 84		Mannitol	62	0.194	0.144	28.538	0.335	38	104	52	90	128	138 duplicate
17449	119 [931; myo-Inositol-2-pho 71		[731; Erythrose (3TMS)]	64	0.191	0.213	9.147	0.390	39	103	44	98	23	100 duplicate
18094	119 [931; myo-Inositol-2-pho 81		Tyrosine	64	0.189	0.318	30.278	0.481	40	102	34	108	133	31 duplicate
19399	119 [931; myo-Inositol-2-pho 110		[715; Erythritol (4TMS)]	54	0.178	0.101	13.025	0.504	41	101	57	85	56	21 duplicate
	135													
9706	119 [931; myo-Inositol-2-pho		[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	0.174	0.340	9.121	0.437	42	100	31	111	22	67 original
9704	119 [931; myo-Inositol-2-pho 133		[855; Squalene]	64	0.171	0.310	7.225	0.335	43	99	35	107	9	137 original
15786	119 [931; myo-Inositol-2-pho 51		[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	0.169	0.166	20.279	0.356	44	98	48	94	109	125 duplicate
18324	119 [931; myo-Inositol-2-pho 85		[529; Methylcitric acid (4TMS)]	48	0.158	0.299	5.802	0.446	45	97	37	105	4	55 duplicate

16704	119 [931; myo-Inositol-2-pho 61 [NA]	64	0.151	0.294	6.289	0.402	46	95	38	104	6	90 duplicate
15963	119 [931; myo-Inositol-2-pho 53 Glycerol-2-phosphate	64	0.151	0.147	12.054	0.405	47	96	51	91	47	88 duplicate
17308	119 [931; myo-Inositol-2-pho 69 Arginine	60	0.149	0.087	18.631	0.493	48	94	58	84	97	28 duplicate
9702	119 [931; myo-Inositol-2-pho 131 [626; 5-Methylthioadenosine (3TMS)]	55	0.143	0.117	17.071	0.508	49	93	55	87	86	20 original
19458	119 [931; myo-Inositol-2-pho 112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.142	0.220	17.864	0.411	50	92	43	99	92	78 duplicate
19123	119 [931; myo-Inositol-2-pho 102 [904; Galactose methoxyamine (5TMS)]	64	0.133	0.143	8.094	0.378	51	91	53	89	17	112 duplicate
18698	119 [931; myo-Inositol-2-pho 92 [680; Glycerol-2-phosphate (4TMS)]	54	0.111	-0.318	11.770	0.455	52	90	127	15	43	49 duplicate
16543	119 [931; myo-Inositol-2-pho 59 Ornithine; Arginine	64	0.107	0.007	37.616	0.368	53	89	72	70	139	121 duplicate
10611	119 [931; myo-Inositol-2-pho 5 Leucine	45	0.099	-0.038	11.668	0.368	54	88	85	57	41	120 duplicate
15605	119 [931; myo-Inositol-2-pho 49 [877; Pyrophosphoric acid (4TMS)]	64	0.098	0.172	20.729	0.432	55	87	48	96	110	71 duplicate
11276	119 [931; myo-Inositol-2-pho 10 Glycine	64	0.097	0.151	15.923	0.516	56	86	50	92	76	13 duplicate
15513	119 [931; myo-Inositol-2-pho 48 Asparagine	56	0.073	0.116	9.981	0.410	58	84	56	86	26	34 duplicate
19598	119 [931; myo-Inositol-2-pho 117 [724; Glycerol (3TMS)]	64	0.065	0.154	7.145	0.365	59	83	49	93	7	122 duplicate
19044	119 [931; myo-Inositol-2-pho 100 [857; Mannitol (6TMS)]	52	0.063	0.271	12.333	0.499	60	82	39	103	48	24 duplicate
12770	119 [931; myo-Inositol-2-pho 22 [690; N,N-Di(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.057	-0.006	20.848	0.379	62	80	75	67	111	110 duplicate
18918	119 [931; myo-Inositol-2-pho 97 [756; beta-D-Methylglucopyranoside (4TMS)]	54	0.054	-0.091	10.622	0.407	63	79	93	49	31	84 original
9891	119 [931; myo-Inositol-2-pho 120 [945; Uridine (3TMS)]	64	0.048	-0.033	27.007	0.370	64	78	81	61	127	117 duplicate
13686	119 [931; myo-Inositol-2-pho 30 [815; Ethyl-3(2H)-thiophenone]	55	0.046	-0.055	13.673	0.407	65	77	89	53	61	85 duplicate
16050	119 [931; myo-Inositol-2-pho 54 [NA]	63	0.036	0.015	17.024	0.387	66	76	69	73	85	106 duplicate
13905	119 [931; myo-Inositol-2-pho 32 [729; N,N-Dimethyllysine methyl ester]	55	0.033	0.022	15.040	0.459	67	74	65	77	71	47 original
9692	119 [931; myo-Inositol-2-pho 121 [657; Erythritol (4TMS)]											
16378	119 [931; myo-Inositol-2-pho 57 [757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55	0.033	-0.034	15.203	0.499	68	75	82	60	73	25 duplicate
14013	119 [931; myo-Inositol-2-pho 33 Methionine	64	0.032	0.012	11.073	0.386	69	73	71	71	36	107 duplicate
12268	119 [931; myo-Inositol-2-pho 18 [590; 1-Acetyl-2-thiohydantoin]	64	0.030	0.032	7.153	0.391	70	72	63	79	8	99 duplicate
11535	119 [931; myo-Inositol-2-pho 12 Glycine acid	63	0.029	0.077	12.489	0.424	71	71	61	81	50	76 duplicate
13236	119 [931; myo-Inositol-2-pho 26 Citramalic acid	64	0.019	0.090	13.171	0.411	72	70	59	83	58	79 duplicate
14331	119 [931; myo-Inositol-2-pho 36 [596; N-Acetylglutamic acid (2TMS)]	64	0.003	-0.007	25.521	0.354	73	69	76	66	121	126 duplicate
17518	119 [931; myo-Inositol-2-pho 72 [919; D-Xylopyranose (4TMS)]	63	-0.002	-0.022	10.886	0.339	74	68	80	62	35	135 duplicate
10880	119 [931; myo-Inositol-2-pho 7 Threonine	41	-0.005	0.025	26.837	0.352	75	67	64	78	126	129 duplicate
18003	119 [931; myo-Inositol-2-pho 99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	64	-0.007	0.121	11.495	0.391	76	66	54	88	39	98 duplicate
14120	119 [931; myo-Inositol-2-pho 34 Aspartic acid	64	-0.011	-0.083	28.734	0.341	77	65	92	50	131	134 duplicate
12651	119 [931; myo-Inositol-2-pho 21 [678; N,N-Di(2-Hydroxyethyl)-methanamine (2TMS)]	64	-0.016	0.022	13.713	0.429	78	64	66	76	62	73 duplicate
11760	119 [931; myo-Inositol-2-pho 14 Fumaric acid	64	-0.019	0.020	10.803	0.408	79	63	67	75	34	83 duplicate
14741	119 [931; myo-Inositol-2-pho 40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	64	-0.021	0.013	31.124	0.442	80	62	70	72	135	60 duplicate
18539	119 [931; myo-Inositol-2-pho 115 Glucose-6-phosphate	62	-0.024	-0.317	22.552	0.495	81	61	126	16	114	27 duplicate
15231	119 [931; myo-Inositol-2-pho 45 Homocysteine	61	-0.026	-0.057	22.647	0.368	82	60	90	52	115	119 duplicate
9700	119 [931; myo-Inositol-2-pho 129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	59	-0.026	-0.016	13.531	0.501	83	59	79	63	59	22 original
13463	119 [931; myo-Inositol-2-pho 28 Malic acid	64	-0.029	0.046	7.634	0.428	84	58	62	80	13	75 duplicate
11013	119 [931; myo-Inositol-2-pho 8 Isoleucine	55	-0.029	0.089	16.669	0.345	85	57	60	82	81	132 duplicate
18211	119 [931; myo-Inositol-2-pho 83 Sorbitol	58	-0.039	-0.055	18.474	0.293	86	56	88	54	95	141 duplicate
15696	119 [931; myo-Inositol-2-pho 50 [746; Ribonic acid-1,4-lactone (3TMS)]	61	-0.051	0.007	19.550	0.397	87	55	73	69	103	95 duplicate
10061	119 [931; myo-Inositol-2-pho 1 [938; Sulfuric acid (2TMS)]	36	-0.060	-0.016	8.928	0.369	88	54	78	64	21	104 duplicate
11145	119 [931; myo-Inositol-2-pho 9 Proline	63	-0.069	-0.011	25.236	0.375	89	53	77	65	120	115 duplicate
19269	119 [931; myo-Inositol-2-pho 106 [733; Threitol (4TMS)]	62	-0.079	-0.188	12.700	0.500	90	52	113	29	54	23 duplicate
13786	119 [931; myo-Inositol-2-pho 31 [622; Parabanic acid (2TMS)]	64	-0.079	-0.118	12.491	0.400	91	50	98	44	51	92 duplicate
16783	119 [931; myo-Inositol-2-pho 62 [812; D-Xylofuranose (4TMS)]	64	-0.079	-0.215	11.893	0.454	92	51	115	27	46	52 duplicate
14226	119 [931; myo-Inositol-2-pho 35 Pyroglutamic acid	64	-0.082	-0.385	38.344	0.533	93	49	130	12	140	7 duplicate
17911	119 [931; myo-Inositol-2-pho 78 Mannose	62	-0.083	-0.180	14.237	0.453	94	48	110	32	64	53 duplicate
17784	119 [931; myo-Inositol-2-pho 76 Fructose	64	-0.084	-0.351	24.263	0.541	95	47	128	14	118	4 duplicate

18486	119 [931; myo-Inositol-2-ph	88	Gluconic acid	64 -0.091	-0.096	12.412	0.520	96	48	94	48	49	10 duplicate
18874	119 [931; myo-Inositol-2-ph	96	myo-Inositol	49 -0.092	-0.001	20.883	0.390	97	45	74	68	112	102 duplicate
14306	119 [931; myo-Inositol-2-ph	11	Succinic acid	64 -0.108	-0.135	7.689	0.404	98	44	102	40	14	88 duplicate
14538	119 [931; myo-Inositol-2-ph	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64 -0.109	-0.037	7.921	0.428	99	43	83	59	15	74 duplicate
9705	119 [931; myo-Inositol-2-ph	134	Isomaltose	64 -0.112	-0.185	24.068	0.536	100	42	111	31	117	6 original
17089	119 [931; myo-Inositol-2-ph	66	Glyceral acid-3-phosphate	64 -0.113	-0.150	8.759	0.341	101	41	105	37	19	133 duplicate
9701	119 [931; myo-Inositol-2-ph	130	Trehalose	63 -0.113	-0.117	26.837	0.372	102	40	97	45	125	116 original
14841	119 [931; myo-Inositol-2-ph	41	[639; Proline (2TMS)]	64 -0.114	-0.110	11.646	0.464	103	39	96	46	40	42 duplicate
15326	119 [931; myo-Inositol-2-ph	46	Arabinose	64 -0.123	-0.252	18.984	0.514	104	38	118	24	100	18 duplicate
10475	119 [931; myo-Inositol-2-ph	4	Phosphoric acid	51 -0.123	-0.041	30.174	0.310	105	37	86	56	132	140 duplicate
10200	119 [931; myo-Inositol-2-ph	2	Serine	62 -0.131	-0.019	17.463	0.365	106	38	68	74	89	123 duplicate
18961	119 [931; myo-Inositol-2-ph	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	48 -0.135	-0.131	20.053	0.330	107	35	101	41	107	139 duplicate
13575	119 [931; myo-Inositol-2-ph	29	Erythritol	64 -0.135	-0.067	7.508	0.420	108	34	91	51	11	77 duplicate
15420	119 [931; myo-Inositol-2-ph	47	[NA]	64 -0.143	-0.180	12.698	0.349	109	33	109	33	53	131 duplicate
18379	119 [931; myo-Inositol-2-ph	86	[793; D-Galactono-1,4-lactone (4TMS)]	61 -0.143	-0.307	23.331	0.562	110	32	123	19	116	2 duplicate
12888	119 [931; myo-Inositol-2-ph	23	Homoserine	64 -0.144	-0.166	11.787	0.402	111	31	107	35	45	89 duplicate
17014	119 [931; myo-Inositol-2-ph	65	[646; 3-Deoxyglucitol (5TMS)]	63 -0.147	-0.168	17.009	0.518	112	30	108	34	84	11 duplicate
19161	119 [931; myo-Inositol-2-ph	103	[648; Ethylamine (2TMS)]	63 -0.149	-0.119	15.653	0.392	113	29	99	43	74	97 duplicate
13350	119 [931; myo-Inositol-2-ph	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53 -0.149	-0.138	19.969	0.356	114	28	103	39	105	124 duplicate
11663	119 [931; myo-Inositol-2-ph	13	Uracil	64 -0.150	-0.110	14.997	0.532	115	27	95	47	70	8 duplicate
9696	119 [931; myo-Inositol-2-ph	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64 -0.155	-0.527	30.390	0.445	116	26	137	5	134	56 original
14640	119 [931; myo-Inositol-2-ph	39	[829; 1-Phenylethanol (1TMS)]	60 -0.156	-0.043	16.149	0.445	117	25	87	55	79	58 duplicate
15038	119 [931; myo-Inositol-2-ph	43	[548; Leucine (2TBS)]	60 -0.159	-0.304	8.865	0.375	118	24	122	20	20	114 duplicate
17719	119 [931; myo-Inositol-2-ph	75	Lysine	64 -0.161	-0.148	36.513	0.352	119	23	104	38	138	127 duplicate
16294	119 [931; myo-Inositol-2-ph	56	[829; Orotic acid (3TMS)]	64 -0.169	-0.251	15.074	0.514	120	21	117	25	72	16 duplicate
12410	119 [931; myo-Inositol-2-ph	19	Alanine (BP)	64 -0.169	-0.276	11.478	0.481	121	22	121	21	38	33 duplicate
19486	119 [931; myo-Inositol-2-ph	113	Galactose-6-phosphate	62 -0.173	-0.427	12.606	0.410	122	20	133	9	52	81 duplicate
17379	119 [931; myo-Inositol-2-ph	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57 -0.182	-0.383	16.811	0.390	123	19	129	13	82	103 duplicate
13005	119 [931; myo-Inositol-2-ph	24	[725; 2-Ketooctanoic acid (2TMS)]	64 -0.186	-0.154	29.365	0.552	124	18	108	36	130	3 duplicate
12041	119 [931; myo-Inositol-2-ph	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64 -0.189	-0.131	15.659	0.523	125	17	100	42	76	9 duplicate
18639	119 [931; myo-Inositol-2-ph	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64 -0.201	-0.198	19.102	0.339	126	16	112	30	101	136 duplicate
19513	119 [931; myo-Inositol-2-ph	114	Fructose-6-phosphate	53 -0.202	-0.315	11.687	0.410	127	15	125	17	42	80 duplicate
18611	119 [931; myo-Inositol-2-ph	118	[928; Glucopyranose-6-phosphate (6TMS)]	58 -0.211	-0.392	11.771	0.397	128	14	131	11	44	94 duplicate
19198	119 [931; myo-Inositol-2-ph	104	[795; Erythritol (4TMS)]	63 -0.212	-0.314	10.369	0.432	129	13	124	18	29	72 duplicate
12165	119 [931; myo-Inositol-2-ph	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64 -0.218	-0.211	16.106	0.399	130	12	114	28	78	93 duplicate
18461	119 [931; myo-Inositol-2-ph	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64 -0.219	-0.265	14.623	0.352	131	11	120	22	67	130 duplicate
19084	119 [931; myo-Inositol-2-ph	101	[832; Dopamine (4TMS)]	64 -0.221	-0.239	13.017	0.383	132	10	118	26	55	108 duplicate
17586	119 [931; myo-Inositol-2-ph	73	[708; Glucose methoxyamine (5TMS)]	57 -0.231	-0.259	13.846	0.462	133	9	119	23	63	45 duplicate
9694	119 [931; myo-Inositol-2-ph	123	[945; Galactofuranose-6-phosphate (7TMS)]	64 -0.242	-0.415	9.993	0.471	134	8	132	10	27	39 original
18433	119 [931; myo-Inositol-2-ph	87	[945; beta-D-Glucopyranose (5TMS)]	62 -0.255	-0.431	33.499	0.390	135	7	134	8	137	101 duplicate
13121	119 [931; myo-Inositol-2-ph	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48 -0.335	-0.499	16.925	0.435	136	6	135	7	83	68 duplicate
10746	119 [931; myo-Inositol-2-ph	6	Glycerol	64 -0.381	-0.591	38.879	0.487	137	5	139	3	141	41 duplicate
18034	119 [931; myo-Inositol-2-ph	80	[772; D-Glucose (5TMS)]	62 -0.390	-0.508	29.208	0.388	138	4	136	6	129	105 duplicate
16938	119 [931; myo-Inositol-2-ph	64	[789; Tyramine (3TMS)]	63 -0.404	-0.527	7.976	0.379	139	3	138	4	16	111 duplicate
17973	119 [931; myo-Inositol-2-ph	79	Glucose	64 -0.446	-0.626	32.828	0.455	140	2	140	2	136	50 duplicate
11916	119 [931; myo-Inositol-2-ph	15	Alanine	64 -0.501	-0.735	17.805	0.482	141	1	141	1	94	30 duplicate
9717	120 [945; Uridine (3TMS)]	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	54 0.550	0.364	21.483	0.521	1	141	11	131	114	61 original
9724	120 [945; Uridine (3TMS)]	132	[895; Isomaltose methoxyamine (8TMS)]	40 0.538	0.309	20.043	0.572	2	140	30	112	103	35 original
16784	120 [945; Uridine (3TMS)]	62	[812; D-Xylofuranose (4TMS)]	54 0.536	0.351	5.536	0.598	3	139	17	125	2	26 duplicate
13464	120 [945; Uridine (3TMS)]	28	Malic acid	54 0.533	0.342	5.750	0.599	4	138	20	122	3	25 duplicate

11407	120 [945; Uridine (3TMS)]	11 Succinic acid	54	0.525	0.386	6.626	0.594	5	137	6	138	9	27 duplicate
11791	120 [945; Uridine (3TMS)]	14 Fumaric acid	54	0.516	0.347	14.457	0.616	6	138	19	123	73	15 duplicate
12652	120 [945; Uridine (3TMS)]	21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	54	0.512	0.457	6.796	0.548	7	135	1	141	11	48 duplicate
13006	120 [945; Uridine (3TMS)]	24 [725; 2-Ketocanoic acid (2TMS)]	54	0.508	0.383	21.167	0.667	8	134	7	135	111	1 duplicate
13576	120 [945; Uridine (3TMS)]	29 Erythritol	54	0.494	0.419	9.773	0.661	10	130	3	139	23	2 duplicate
14742	120 [945; Uridine (3TMS)]	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	54	0.494	0.364	22.233	0.558	11	131	10	132	120	42 duplicate
14539	120 [945; Uridine (3TMS)]	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	54	0.494	0.359	7.135	0.651	12	132	14	128	12	4 duplicate
15327	120 [945; Uridine (3TMS)]	46 Arabinose	54	0.493	0.342	12.310	0.636	13	129	21	121	47	8 duplicate
18487	120 [945; Uridine (3TMS)]	88 Gluconic acid	54	0.488	0.328	8.541	0.591	14	128	25	117	18	28 duplicate
14641	120 [945; Uridine (3TMS)]	39 [829; 1-Phenylethanol (1TMS)]	54	0.480	0.363	10.932	0.642	15	127	13	129	37	7 duplicate
18380	120 [945; Uridine (3TMS)]	86 [793; D-Galactono-1,4-lactone (4TMS)]	51	0.478	0.323	16.001	0.631	16	126	27	115	81	11 duplicate
12042	120 [945; Uridine (3TMS)]	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	54	0.477	0.412	8.442	0.648	17	125	4	138	17	5 duplicate
14227	120 [945; Uridine (3TMS)]	35 Pyroglutamic acid	54	0.474	0.256	29.127	0.508	18	124	39	103	139	67 duplicate
17015	120 [945; Uridine (3TMS)]	65 [646; 3-Deoxyglucitol (5TMS)]	54	0.473	0.350	14.284	0.635	19	123	18	124	69	9 duplicate
11536	120 [945; Uridine (3TMS)]	12 Glyceric acid	54	0.470	0.380	16.265	0.604	20	121	8	134	86	22 duplicate
17785	120 [945; Uridine (3TMS)]	76 Fructose	54	0.470	0.300	16.130	0.554	21	122	31	111	84	45 duplicate
9721	120 [945; Uridine (3TMS)]	129 [840; Maltose methoxamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	54	0.465	0.338	13.408	0.586	22	120	23	119	60	29 original
19124	120 [945; Uridine (3TMS)]	102 [904; Galactose methoxamine (5TMS)]	54	0.463	0.232	11.635	0.571	23	119	44	98	42	36 duplicate
13237	120 [945; Uridine (3TMS)]	26 Citramalic acid	54	0.462	0.426	6.365	0.554	24	118	2	140	6	46 duplicate
19270	120 [945; Uridine (3TMS)]	106 [733; Threitol (4TMS)]	53	0.462	0.292	9.939	0.615	25	117	32	110	27	16 duplicate
19540	120 [945; Uridine (3TMS)]	115 Glucose-6-phosphate	54	0.458	0.225	14.800	0.570	26	116	46	98	75	37 duplicate
12771	120 [945; Uridine (3TMS)]	22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	48	0.456	0.282	17.396	0.609	27	115	34	108	91	20 duplicate
15697	120 [945; Uridine (3TMS)]	50 [746; Ribonic acid-1,4-lactone (3TMS)]	53	0.453	0.388	23.676	0.610	28	114	5	137	128	19 duplicate
16379	120 [945; Uridine (3TMS)]	57 [757; 2-Desoxy-pentose-3-yose dimethoxamine (2TMS)]	51	0.451	0.320	12.840	0.609	29	113	28	114	56	21 duplicate
16295	120 [945; Uridine (3TMS)]	56 [829; Orolic acid (3TMS)]	54	0.449	0.341	13.166	0.618	30	112	22	120	59	14 duplicate
18325	120 [945; Uridine (3TMS)]	85 [528; Methylcitric acid (4TMS)]	38	0.448	0.354	7.479	0.509	31	111	16	126	15	65 duplicate
9728	120 [945; Uridine (3TMS)]	134 Isomaltose	54	0.444	0.329	16.806	0.654	32	110	24	118	88	3 original
16051	120 [945; Uridine (3TMS)]	54 [NA]	48	0.443	0.325	14.874	0.545	33	109	26	116	77	50 duplicate
11664	120 [945; Uridine (3TMS)]	13 Uracil	54	0.438	0.364	8.702	0.644	34	108	12	130	19	6 duplicate
17380	120 [945; Uridine (3TMS)]	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	48	0.436	0.214	10.148	0.401	35	107	50	82	29	108 duplicate
17654	120 [945; Uridine (3TMS)]	74 [912; Tetradecanoic acid (1TMS)]	54	0.434	0.265	13.489	0.486	36	106	38	104	61	74 duplicate
19045	120 [945; Uridine (3TMS)]	112 [877; Mannitol (6TMS)]	54	0.433	0.278	6.166	0.567	37	104	35	107	5	39 duplicate
19459	120 [945; Uridine (3TMS)]	100 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	54	0.433	0.191	22.233	0.528	38	105	52	90	119	58 duplicate
17912	120 [945; Uridine (3TMS)]	117 [724; Glyceral (3TMS)]	52	0.425	0.283	13.725	0.512	39	103	33	109	63	63 duplicate
19589	120 [945; Uridine (3TMS)]	78 Mannose	51	0.420	0.228	12.863	0.552	40	102	45	97	57	47 duplicate
9714	120 [945; Uridine (3TMS)]	122 [644; Erythritol (4TMS)]	48	0.399	0.240	20.438	0.569	41	101	42	100	108	38 original
12166	120 [945; Uridine (3TMS)]	17 [700; 2-methyl-1,2-propanediol (2TMS)]	54	0.398	0.358	8.870	0.575	42	100	15	127	21	34 duplicate
19400	120 [945; Uridine (3TMS)]	110 [715; Erythritol (4TMS)]	48	0.394	0.216	15.112	0.612	43	99	49	93	79	18 duplicate
9727	120 [945; Uridine (3TMS)]	135	54	0.391	0.169	5.092	0.474	44	98	61	81	1	75 original
15136	120 [945; Uridine (3TMS)]	44 [910; 2-Ketogluconic acid methoxamine (4TMS)]	45	0.356	0.253	9.842	0.578	45	97	40	102	24	31 duplicate
12289	120 [945; Uridine (3TMS)]	18 [590; 1-Acetyl-2-thiohydantoin]	54	0.352	0.314	7.207	0.446	46	96	29	113	13	92 duplicate
9713	120 [945; Uridine (3TMS)]	121 [657; Erythritol (4TMS)]	47	0.349	0.184	18.313	0.528	47	95	55	87	95	59 original
9718	120 [945; Uridine (3TMS)]	126 [559; Erythritol (4TMS)]	44	0.347	0.070	13.769	0.577	48	94	72	70	65	32 original
18689	120 [945; Uridine (3TMS)]	82 [680; Glyceral-2-phosphate (4TMS)]	49	0.332	0.176	11.643	0.488	49	93	59	83	43	72 duplicate
19004	120 [945; Uridine (3TMS)]	99 [662; Ribose-5-phosphate methoxamine (BP) (5TMS)]	39	0.323	0.265	15.180	0.581	50	92	37	105	80	30 duplicate
17587	120 [945; Uridine (3TMS)]	73 [708; Glucose methoxamine (5TMS)]	47	0.319	0.223	12.485	0.456	51	91	47	95	49	83 duplicate
19162	120 [945; Uridine (3TMS)]	103 [648; Ethylamine (2TMS)]	54	0.290	0.183	12.803	0.509	52	90	56	86	54	66 duplicate
19487	120 [945; Uridine (3TMS)]	113 Galactose-6-phosphate	54	0.282	0.172	12.647	0.449	53	89	60	82	63	89 duplicate

10747	120 [945; Uridine (3TMS)]	6	Glycerol	54	0.276	0.266	29,354	0.447	54	88	36	106	140	91	duplicate
19514	120 [945; Uridine (3TMS)]	114	Fructose-6-phosphate	48	0.261	0.137	13,666	0.449	55	87	65	77	62	88	duplicate
18240	120 [945; Uridine (3TMS)]	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	43	0.258	0.047	8,792	0.533	56	88	74	68	20	56	original
16434	120 [945; Uridine (3TMS)]	87	[945; beta-D-Glucopyranose (5TMS)]	52	0.240	0.191	24,542	0.466	57	85	53	89	130	81	duplicate
18919	120 [945; Uridine (3TMS)]	97	[756; beta-D-Methylglucopyranoside (4TMS)]	49	0.235	0.196	16,043	0.441	58	84	51	91	82	96	duplicate
12411	120 [945; Uridine (3TMS)]	19	Alanine (BP) (3TMS)	54	0.226	0.137	7,302	0.468	59	83	68	78	14	78	duplicate
19565	120 [945; Uridine (3TMS)]	116	[882; Pseudouridine (5TMS)]	27	0.225	0.077	11,861	0.292	60	82	70	72	45	140	duplicate
19235	120 [945; Uridine (3TMS)]	105	[705; 2-Ketogluconic acid (5TMS)]	45	0.224	0.182	11,516	0.511	61	81	57	85	41	64	duplicate
18640	120 [945; Uridine (3TMS)]	91	[766; beta-D-Methylglucopyranoside (4TMS)]	54	0.212	0.188	16,123	0.407	62	79	54	88	83	106	duplicate
14842	120 [945; Uridine (3TMS)]	41	[639; Proline (2TMS)]	54	0.212	0.096	6,668	0.451	63	80	69	73	10	86	duplicate
18875	120 [945; Uridine (3TMS)]	96	myo-Inositol	40	0.197	0.043	23,157	0.228	64	78	75	67	125	141	duplicate
19199	120 [945; Uridine (3TMS)]	104	[785; Erythritol (4TMS)]	53	0.194	0.180	10,293	0.426	65	77	58	84	31	99	duplicate
19085	120 [945; Uridine (3TMS)]	101	[832; Dopamine (4TMS)]	54	0.185	0.141	11,153	0.434	66	76	63	79	39	97	duplicate
10062	120 [945; Uridine (3TMS)]	1	[938; Sulfuric acid (2TMS)]	33	0.167	0.241	11,844	0.534	67	75	41	101	44	55	duplicate
18269	120 [945; Uridine (3TMS)]	84	Mannitol	52	0.166	0.219	21,471	0.462	68	74	48	94	113	82	duplicate
9732	120 [945; Uridine (3TMS)]	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	40	0.162	0.100	20,131	0.393	69	73	68	74	104	115	original
19369	120 [945; Uridine (3TMS)]	109	Octadecanoic acid	54	0.152	0.049	15,054	0.412	70	72	73	69	78	102	duplicate
9719	120 [945; Uridine (3TMS)]	127	[777; Fructose-6-phosphate methoxymine (6TMS)]	38	0.147	-0.023	10,434	0.521	71	71	81	61	32	60	original
15964	120 [945; Uridine (3TMS)]	53	Glycerol-2-phosphate	54	0.131	0.232	17,221	0.357	72	70	43	99	80	127	duplicate
18212	120 [945; Uridine (3TMS)]	48	Octadecanoic acid	48	0.126	-0.280	12,624	0.357	73	69	112	30	52	128	duplicate
15421	120 [945; Uridine (3TMS)]	47	[NA]	54	0.124	0.135	12,828	0.447	74	68	67	75	55	90	duplicate
16784	120 [945; Uridine (3TMS)]	94	Hexadecanoic acid	54	0.114	0.013	12,444	0.444	75	67	79	63	48	94	duplicate
9715	120 [945; Uridine (3TMS)]	123	[945; Galactofuranose-6-phosphate (7TMS)]	54	0.113	0.035	6,377	0.434	76	66	76	66	7	98	original
9725	120 [945; Uridine (3TMS)]	141	Lanosta-8,24-dien-3-beta-ol	51	0.108	0.009	19,746	0.417	77	65	80	62	102	101	original
18035	120 [945; Uridine (3TMS)]	133	[855; Squalene]	54	0.100	-0.084	11,010	0.398	78	64	87	55	38	111	original
16590	120 [945; Uridine (3TMS)]	80	[772; D-Glucose (5TMS)]	52	0.083	0.137	20,437	0.407	79	63	64	78	107	105	duplicate
11917	120 [945; Uridine (3TMS)]	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	54	0.082	-0.024	9,370	0.342	80	62	82	60	22	132	duplicate
19430	120 [945; Uridine (3TMS)]	15	Alanine	54	0.071	0.015	9,911	0.566	81	61	77	65	26	40	duplicate
19634	120 [945; Uridine (3TMS)]	111	[583; Erythritol (4TMS)]	38	0.064	-0.076	24,741	0.325	82	60	86	56	131	135	duplicate
17874	120 [945; Uridine (3TMS)]	119	[931; myo-Inositol-2-phosphate (7TMS)]	54	0.054	-0.091	10,622	0.407	83	59	88	54	33	104	duplicate
9730	120 [945; Uridine (3TMS)]	79	Glucose	54	0.044	0.159	23,585	0.491	84	58	62	80	126	71	duplicate
16939	120 [945; Uridine (3TMS)]	138	[674; Ergosterol (1TMS)]	39	0.038	-0.122	21,158	0.363	85	57	93	49	110	124	original
9729	120 [945; Uridine (3TMS)]	64	[789; Tyramine (3TMS)]	54	0.030	-0.043	10,745	0.399	86	56	84	58	35	109	duplicate
18737	120 [945; Uridine (3TMS)]	93	Ergosterol	54	0.027	-0.105	10,658	0.367	87	55	89	53	34	123	original
19304	120 [945; Uridine (3TMS)]	107	9-(Z)-Octadecenoic acid	53	0.025	-0.118	22,564	0.352	88	54	91	51	122	130	duplicate
17519	120 [945; Uridine (3TMS)]	72	[919; D-Xylopyranose (4TMS)]	54	0.019	-0.138	6,451	0.359	89	53	97	45	8	126	duplicate
9731	120 [945; Uridine (3TMS)]	139	[700; Ergosta-5,7-dien-3-ol]	53	0.001	0.077	14,325	0.347	90	52	71	70	131	duplicate	
19612	120 [945; Uridine (3TMS)]	118	[928; Glucopyranose-6-phosphate (6TMS)]	32	-0.004	-0.109	22,213	0.318	91	51	90	52	118	137	original
9716	120 [945; Uridine (3TMS)]	124	[734; 1-Monoolioglycerol (2TMS); 1-Monohexadecenylglycerol (1TMS)]	53	-0.035	-0.070	14,325	0.388	92	50	85	57	71	118	duplicate
17450	120 [945; Uridine (3TMS)]	71	[731; Erythrose (3TMS)]	49	-0.044	-0.147	28,974	0.392	93	49	99	43	138	116	original
19337	120 [945; Uridine (3TMS)]	108	Octadecenoic acid	54	-0.075	-0.135	5,617	0.410	94	48	96	46	4	103	duplicate
9722	120 [945; Uridine (3TMS)]	130	Trehalose	54	-0.110	-0.131	17,939	0.395	96	46	95	47	94	114	original
10476	120 [945; Uridine (3TMS)]	4	Phosphoric acid	41	-0.112	-0.214	21,561	0.316	97	45	103	39	115	138	duplicate
14332	120 [945; Uridine (3TMS)]	36	[596; N-Acetylglylamic acid (2TMS)]	54	-0.115	-0.128	17,166	0.382	98	44	94	48	89	120	duplicate
16862	120 [945; Uridine (3TMS)]	52	[NA]	39	-0.117	-0.282	25,588	0.556	99	43	113	29	133	44	duplicate
18539	120 [945; Uridine (3TMS)]	63	Glutamine	43	-0.132	-0.143	19,429	0.632	100	42	98	44	100	10	duplicate
17090	120 [945; Uridine (3TMS)]	89	[775; Dopamine (4TMS)]	27	-0.185	-0.120	18,926	0.328	101	41	92	50	98	134	duplicate
18982	120 [945; Uridine (3TMS)]	98	[697; Ribose-5-phosphate methoxymine (5TMS)]	54	-0.203	-0.182	12,890	0.560	102	40	101	41	58	41	duplicate
				39	-0.223	-0.035	23,018	0.557	103	39	83	59	123	43	duplicate

16462	120 [945; Uridine (3TMS)]	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	54 -0.234	-0.236	9,970	0.334	104	38	107	35	28	133 duplicate
17164	120 [945; Uridine (3TMS)]	67 Citric acid	54 -0.241	-0.270	12,591	0.362	105	37	111	31	51	125 duplicate
15787	120 [945; Uridine (3TMS)]	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	36 -0.251	-0.224	23,089	0.494	106	36	104	38	124	70 duplicate
17720	120 [945; Uridine (3TMS)]	75 Lysine	54 -0.258	-0.339	26,836	0.369	107	35	121	21	135	122 duplicate
9728	120 [945; Uridine (3TMS)]	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	16 -0.267	-0.524	7,669	0.319	108	34	140	2	16	138 original
13351	120 [945; Uridine (3TMS)]	27 [815; (E)-4-Methyl-5-hydroxy-3-pentan-2-one (1TMS)]	43 -0.267	-0.226	23,611	0.538	109	33	105	37	127	53 duplicate
17237	120 [945; Uridine (3TMS)]	68 [570; Hypoxanthine (2TMS)]	15 -0.276	-0.300	16,777	0.397	110	32	114	28	87	112 duplicate
16825	120 [945; Uridine (3TMS)]	60 Glycerol-3-phosphate	54 -0.279	-0.313	11,251	0.424	111	31	115	27	40	100 duplicate
11014	120 [945; Uridine (3TMS)]	8 Isoleucine	45 -0.287	-0.322	14,849	0.306	112	30	118	24	76	139 duplicate
16705	120 [945; Uridine (3TMS)]	61 [NA]	54 -0.289	-0.262	10,227	0.472	113	29	110	32	30	78 duplicate
13122	120 [945; Uridine (3TMS)]	25 [709; 2,5-Diaminovalerolactam (2TMS)]	45 -0.297	-0.226	20,350	0.612	114	28	106	36	105	77 duplicate
10339	120 [945; Uridine (3TMS)]	3 Ethanolamine	52 -0.299	-0.251	17,725	0.444	115	27	109	33	93	95 duplicate
15039	120 [945; Uridine (3TMS)]	43 [548; Leucine (2TBS)]	50 -0.300	-0.208	9,843	0.398	116	26	102	40	25	110 duplicate
10201	120 [945; Uridine (3TMS)]	2 Serine	52 -0.309	-0.411	16,174	0.396	117	25	129	13	85	113 duplicate
12889	120 [945; Uridine (3TMS)]	23 Homoserine	54 -0.312	-0.330	13,767	0.604	118	24	120	22	64	23 duplicate
10881	120 [945; Uridine (3TMS)]	7 Threonine	54 -0.314	-0.355	18,453	0.354	119	23	124	18	97	129 duplicate
9723	120 [945; Uridine (3TMS)]	131 [626; 5-Methylthiodenosine (3TMS)]	45 -0.321	-0.014	21,687	0.513	120	22	78	64	116	62 original
14436	120 [945; Uridine (3TMS)]	37 Phenylalanine	54 -0.350	-0.385	12,056	0.469	121	21	127	15	46	77 duplicate
15606	120 [945; Uridine (3TMS)]	49 [877; Pyrophosphoric acid (4TMS)]	54 -0.352	-0.368	26,727	0.444	122	20	125	17	134	93 duplicate
11146	120 [945; Uridine (3TMS)]	9 Proline	53 -0.357	-0.431	20,394	0.391	123	19	135	7	106	117 duplicate
10612	120 [945; Uridine (3TMS)]	5 Leucine	35 -0.358	-0.248	14,196	0.545	124	18	108	34	67	49 duplicate
13906	120 [945; Uridine (3TMS)]	32 [729; N,N-Dimethyllysine methyl ester]	53 -0.358	-0.416	22,521	0.600	125	17	130	12	121	24 duplicate
12532	120 [945; Uridine (3TMS)]	20 [619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	23 -0.368	-0.374	18,427	0.536	126	16	126	16	96	54 duplicate
18095	120 [945; Uridine (3TMS)]	81 Tyrosine	54 -0.381	-0.355	21,848	0.530	127	15	123	19	117	57 duplicate
17309	120 [945; Uridine (3TMS)]	69 Arginine	50 -0.388	-0.419	14,204	0.620	128	14	131	11	68	13 duplicate
14121	120 [945; Uridine (3TMS)]	34 Aspartic acid	54 -0.388	-0.426	21,321	0.453	129	13	133	9	112	85 duplicate
14014	120 [945; Uridine (3TMS)]	33 Methionine	54 -0.396	-0.439	14,380	0.468	130	12	138	4	72	79 duplicate
13687	120 [945; Uridine (3TMS)]	30 [815; Ethyl-3-(2H)-thiophenone]	54 -0.398	-0.424	19,509	0.402	131	11	132	10	101	107 duplicate
16137	120 [945; Uridine (3TMS)]	55 [612; 4-Aminobutyric acid (2TBS)]	33 -0.398	-0.324	24,905	0.456	132	10	119	23	132	84 duplicate
15514	120 [945; Uridine (3TMS)]	48 Asparagine	54 -0.399	-0.317	14,537	0.577	133	9	116	28	74	33 duplicate
11277	120 [945; Uridine (3TMS)]	10 Glycine	54 -0.400	-0.320	10,870	0.623	134	8	117	25	36	12 duplicate
18830	120 [945; Uridine (3TMS)]	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	40 -0.403	-0.478	24,417	0.374	135	7	139	3	129	121 duplicate
13797	120 [945; Uridine (3TMS)]	31 [622; Parabanic acid (2TMS)]	54 -0.405	-0.436	17,707	0.541	136	6	136	6	92	52 duplicate
15232	120 [945; Uridine (3TMS)]	45 Homocysteine	51 -0.405	-0.351	27,130	0.451	137	5	122	20	136	87 duplicate
14941	120 [945; Uridine (3TMS)]	42 Glutamic acid	50 -0.408	-0.438	21,026	0.467	138	4	137	5	109	80 duplicate
16544	120 [945; Uridine (3TMS)]	59 Ornithine; Arginine	54 -0.433	-0.428	27,864	0.504	139	3	134	8	137	68 duplicate
18154	120 [945; Uridine (3TMS)]	82 Lysine	30 -0.444	-0.406	12,555	0.542	140	2	128	14	50	51 duplicate
17849	120 [945; Uridine (3TMS)]	[826; beta-[(5-methyl-2-thienyl)methyleneamino]-benzeneacetic acid methyl ester]	52 -0.498	-0.559	19,403	0.497	141	1	141	1	89	69 duplicate
19590	121 [657; Erythritol (4TMS)]	117 [724; Glycerol (3TMS)]	50 0.886	0.962	8,905	0.673	1	141	1	141	19	2 duplicate
19401	121 [657; Erythritol (4TMS)]	110 [715; Erythritol (4TMS)]	51 0.878	0.946	7,645	0.651	2	140	3	139	15	3 duplicate
9734	121 [657; Erythritol (4TMS)]	122 [844; Erythritol (4TMS)]	48 0.876	0.933	4,516	0.632	3	139	4	138	2	8 original
19271	121 [657; Erythritol (4TMS)]	108 [733; Threitol (4TMS)]	53 0.837	0.955	14,854	0.678	4	138	2	140	59	1 duplicate
15137	121 [657; Erythritol (4TMS)]	44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	47 0.796	0.918	11,980	0.650	5	137	6	136	43	4 duplicate
9738	121 [657; Erythritol (4TMS)]	126 [559; Erythritol (4TMS)]	44 0.793	0.933	5,500	0.629	6	136	5	137	4	9 original
17786	121 [657; Erythritol (4TMS)]	76 Fructose	55 0.756	0.837	32,708	0.601	7	135	8	134	120	18 duplicate
14743	121 [657; Erythritol (4TMS)]	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	55 0.725	0.895	41,281	0.617	8	134	7	135	135	12 duplicate
19541	121 [657; Erythritol (4TMS)]	115 Glucose-6-phosphate	53 0.694	0.816	31,812	0.590	9	133	11	131	118	23 duplicate
17588	121 [657; Erythritol (4TMS)]	73 [708; Glucose methoxyamine (5TMS)]	48 0.651	0.834	9,518	0.538	10	132	9	133	23	49 duplicate

17913	121 [657; Erythritol (4TMS)]	78 Mannose	53 0.650	0.827	9.431	0.575	11	131	10	132	22	33 duplicate
14228	121 [657; Erythritol (4TMS)]	35 Pyroglutamic acid	55 0.644	0.774	48.054	0.597	12	130	17	125	140	20 duplicate
13465	121 [657; Erythritol (4TMS)]	28 Malic acid	55 0.605	0.814	16.897	0.566	13	129	12	130	74	36 duplicate
19046	121 [657; Erythritol (4TMS)]	100 [657; Mannitol (6TMS)]	55 0.595	0.695	16.410	0.524	14	128	37	105	68	60 duplicate
11792	121 [657; Erythritol (4TMS)]	14 Fumaric acid	55 0.562	0.779	7.525	0.580	15	127	14	128	11	30 duplicate
18381	121 [657; Erythritol (4TMS)]	86 [793; D-Galactono-1,4-lactone (4TMS)]	52 0.540	0.780	26.380	0.647	16	126	13	129	107	5 duplicate
19488	121 [657; Erythritol (4TMS)]	113 Galactose-6-phosphate	53 0.528	0.743	9.170	0.563	17	125	22	120	21	38 duplicate
14540	121 [657; Erythritol (4TMS)]	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	55 0.526	0.775	14.793	0.598	18	124	16	126	58	19 duplicate
12772	121 [657; Erythritol (4TMS)]	22 [690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	45 0.525	0.731	4.931	0.582	19	123	28	116	3	28 duplicate
19125	121 [657; Erythritol (4TMS)]	102 [904; Galactose methoxyamine (5TMS)]	55 0.522	0.632	10.268	0.548	20	122	47	95	26	41 duplicate
13238	121 [657; Erythritol (4TMS)]	26 Citramalic acid	55 0.521	0.723	24.135	0.520	21	121	30	112	100	63 duplicate
17655	121 [657; Erythritol (4TMS)]	74 [912; Tetradecanoic acid (1TMS)]	55 0.516	0.770	11.247	0.485	22	120	18	124	33	79 duplicate
18515	121 [657; Erythritol (4TMS)]	114 Fructose-6-phosphate	46 0.511	0.764	7.010	0.587	23	119	19	123	8	25 duplicate
14642	121 [657; Erythritol (4TMS)]	39 [829; 1-Phenylethanol (1TMS)]	54 0.501	0.777	22.159	0.613	24	118	15	127	94	14 duplicate
17381	121 [657; Erythritol (4TMS)]	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	48 0.500	0.555	25.351	0.528	25	117	58	84	103	56 duplicate
16785	121 [657; Erythritol (4TMS)]	62 [812; D-Xylofuranose (4TMS)]	55 0.481	0.704	22.074	0.590	26	116	34	108	92	22 duplicate
12412	121 [657; Erythritol (4TMS)]	19 Alanine (BP) (3TMS)	55 0.475	0.727	18.917	0.514	27	115	28	114	86	65 duplicate
9747	121 [657; Erythritol (4TMS)]	135	55 0.469	0.603	20.132	0.459	28	114	51	91	89	92 original
12653	121 [657; Erythritol (4TMS)]	21 [678; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	55 0.468	0.653	24.297	0.525	29	113	42	100	101	57 duplicate
19200	121 [657; Erythritol (4TMS)]	104 [795; Erythritol (4TMS)]	54 0.468	0.759	12.380	0.564	30	112	21	121	47	37 duplicate
16296	121 [657; Erythritol (4TMS)]	56 [829; Orolic acid (3TMS)]	55 0.457	0.726	11.274	0.602	31	111	29	113	34	17 duplicate
13577	121 [657; Erythritol (4TMS)]	29 Erythritol	55 0.453	0.693	11.780	0.556	32	109	38	104	40	39 duplicate
11408	121 [657; Erythritol (4TMS)]	11 Succinic acid	55 0.453	0.693	15.161	0.544	33	110	39	103	63	44 duplicate
13007	121 [657; Erythritol (4TMS)]	24 [725; 2-Ketocanoic acid (2TMS)]	55 0.448	0.732	39.410	0.626	34	108	25	117	132	10 duplicate
17016	121 [657; Erythritol (4TMS)]	65 [646; 3-Deoxyglucitol (5TMS)]	54 0.442	0.761	12.894	0.614	35	106	20	122	51	13 duplicate
15698	121 [657; Erythritol (4TMS)]	50 [746; Ribonic acid-1,4-lactone (3TMS)]	54 0.442	0.696	6.898	0.548	36	107	36	106	7	42 duplicate
12290	121 [657; Erythritol (4TMS)]	18 [590; 1-Acetyl-2-thiohydantoin]	55 0.432	0.633	15.019	0.491	37	105	46	96	60	76 duplicate
9746	121 [657; Erythritol (4TMS)]	134 Isomaltose	55 0.426	0.739	32.186	0.619	38	103	23	119	119	11 original
12043	121 [657; Erythritol (4TMS)]	16 [844; 2-Methyl-1,3-butanediol (2TMS)]	55 0.424	0.705	25.555	0.640	40	102	33	109	106	6 duplicate
19460	121 [657; Erythritol (4TMS)]	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	54 0.421	0.580	7.182	0.476	41	101	53	89	10	85 duplicate
11665	121 [657; Erythritol (4TMS)]	13 Uracil	55 0.421	0.710	23.659	0.635	42	99	32	110	99	7 duplicate
9737	121 [657; Erythritol (4TMS)]	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	55 0.421	0.631	39.366	0.552	43	100	48	94	131	40 original
18326	121 [657; Erythritol (4TMS)]	85 [529; Methylcitric acid (4TMS)]	39 0.417	0.711	10.750	0.497	44	98	31	111	28	74 duplicate
14843	121 [657; Erythritol (4TMS)]	41 [639; Proline (2TMS)]	55 0.415	0.642	20.965	0.502	45	98	45	87	91	72 duplicate
9735	121 [657; Erythritol (4TMS)]	123 [945; Galactofuranose-6-phosphate (7TMS)]	55 0.415	0.608	18.597	0.492	46	97	50	92	84	75 original
15328	121 [657; Erythritol (4TMS)]	46 Arabinose	55 0.405	0.728	22.936	0.605	47	95	27	115	96	16 duplicate
11537	121 [657; Erythritol (4TMS)]	12 Glyceric acid	54 0.405	0.648	6.417	0.527	48	94	43	99	5	55 duplicate
9741	121 [657; Erythritol (4TMS)]	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	52 0.397	0.702	13.808	0.587	49	93	35	107	55	24 original
18488	121 [657; Erythritol (4TMS)]	88 Gluconic acid	55 0.386	0.610	18.756	0.581	50	92	49	83	85	29 duplicate
10748	121 [657; Erythritol (4TMS)]	6 Glycerol	55 0.376	0.594	48.420	0.586	51	91	52	90	141	26 duplicate
12167	121 [657; Erythritol (4TMS)]	17 [700; 2-methyl-1,2-propanediol (2TMS)]	55 0.372	0.659	25.386	0.545	52	90	40	102	104	43 duplicate
9739	121 [657; Erythritol (4TMS)]	127 [777; Fructose-6-phosphate methoxyamine (6TMS)]	39 0.360	0.445	8.290	0.492	53	89	63	79	18	81 original
19163	121 [657; Erythritol (4TMS)]	103 [648; Ethylamine (2TMS)]	55 0.351	0.451	19.759	0.441	54	88	62	80	87	100 duplicate
19656	121 [657; Erythritol (4TMS)]	120 [945; Uridine (3TMS)]	47 0.349	0.184	18.313	0.528	55	87	78	64	81	53 duplicate
16380	121 [657; Erythritol (4TMS)]	57 [757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	49 0.349	0.654	17.272	0.584	56	86	41	101	76	27 duplicate
18213	121 [657; Erythritol (4TMS)]	83 Sorbitol	49 0.316	0.159	27.379	0.312	57	85	81	61	111	139 duplicate
9744	121 [657; Erythritol (4TMS)]	132 [895; Isomaltose methoxyamine (8TMS)]	37 0.315	0.558	7.542	0.588	58	84	57	85	12	35 original
19370	121 [657; Erythritol (4TMS)]	109 Octadecanoic acid	55 0.302	0.732	28.067	0.524	59	83	24	118	112	58 duplicate



18690	121 [657; Erythritol (4TMS)]	82 [680; Glycerol-2-phosphate (4TMS)]	49 0.301	0.427	11.784	0.521	60	82	64	78	41	62 duplicate
9740	121 [657; Erythritol (4TMS)]	128 [924; D-Sedoheptulose-7-phosphate (7TMS)]	42 0.292	0.398	12.676	0.512	61	81	67	75	49	69 original
9752	121 [657; Erythritol (4TMS)]	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	41 0.288	0.393	7.605	0.391	62	80	68	74	13	122 original
18785	121 [657; Erythritol (4TMS)]	94 Hexadecanoic acid	55 0.279	0.846	28.172	0.527	63	78	44	98	113	64 duplicate
19086	121 [657; Erythritol (4TMS)]	101 [832; Dopamine (4TMS)]	55 0.279	0.308	16.974	0.387	64	79	72	70	75	124 duplicate
18435	121 [657; Erythritol (4TMS)]	87 [945; beta-D-Glucopyranose (5TMS)]	53 0.279	0.564	41.820	0.514	65	77	56	86	136	66 duplicate
19431	121 [657; Erythritol (4TMS)]	111 [583; Erythritol (4TMS)]	39 0.260	0.316	11.735	0.453	66	76	71	71	38	95 duplicate
19566	121 [657; Erythritol (4TMS)]	116 [882; Pseudouridine (5TMS)]	24 0.254	0.568	6.620	0.464	67	75	55	87	6	90 duplicate
9750	121 [657; Erythritol (4TMS)]	138 [674; Ergosterol (1TMS)]	38 0.243	0.400	8.053	0.400	68	74	66	76	17	119 original
9736	121 [657; Erythritol (4TMS)]	133 [855; Squalene]	55 0.239	0.288	14.176	0.360	69	73	74	68	57	131 original
19235	121 [657; Erythritol (4TMS)]	105 [705; 2-Ketogluconic acid (5TMS)]	46 0.239	0.344	16.412	0.471	70	72	70	72	69	89 duplicate
16052	121 [657; Erythritol (4TMS)]	54 [NA]	48 0.215	0.478	8.045	0.540	71	71	59	83	16	47 duplicate
9753	121 [657; Erythritol (4TMS)]	141 Lanosta-8,24-dien-3-beta-ol	52 0.214	0.357	7.625	0.410	72	70	69	73	14	112 original
18876	121 [657; Erythritol (4TMS)]	96 myo-Inositol	40 0.208	0.213	10.186	0.317	73	69	76	66	25	137 duplicate
17975	121 [657; Erythritol (4TMS)]	79 Glucose	55 0.195	0.473	42.367	0.539	74	68	60	82	137	48 duplicate
18036	121 [657; Erythritol (4TMS)]	80 [772; D-Glucose (5TMS)]	53 0.171	0.452	37.733	0.474	75	67	61	81	128	87 duplicate
17451	121 [657; Erythritol (4TMS)]	71 [731; Erythrose (3TMS)]	55 0.157	0.298	19.944	0.426	76	66	73	69	88	105 duplicate
18920	121 [657; Erythritol (4TMS)]	97 [756; beta-D-Methylglucopyranoside (4TMS)]	48 0.144	0.178	26.984	0.451	77	65	79	63	110	97 duplicate
18641	121 [657; Erythritol (4TMS)]	91 [766; beta-D-Methylglucopyranoside (4TMS)]	55 0.118	0.099	22.938	0.404	78	64	84	58	97	116 duplicate
9749	121 [657; Erythritol (4TMS)]	137 Ergosterol	55 0.116	0.145	20.914	0.402	79	63	82	80	90	118 original
19613	121 [657; Erythritol (4TMS)]	118 [928; Glucopyranose-6-phosphate (6TMS)]	51 0.111	0.247	10.507	0.440	80	62	75	67	27	101 duplicate
9748	121 [657; Erythritol (4TMS)]	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17 0.103	0.213	4.203	0.421	81	61	77	65	1	106 original
16940	121 [657; Erythritol (4TMS)]	64 [789; Tyramine (3TMS)]	54 0.098	0.121	11.920	0.412	82	60	83	59	42	110 duplicate
11918	121 [657; Erythritol (4TMS)]	15 Alanine	55 0.048	0.166	26.569	0.541	83	59	80	62	108	46 duplicate
		124 [734; 1-Monooctyleoglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]										
9736	121 [657; Erythritol (4TMS)]	119 [931; myo-Inositol-2-phosphate (7TMS)]	50 0.033	0.018	13.161	0.403	84	58	86	56	53	117 original
18635	121 [657; Erythritol (4TMS)]	139 [700; Ergosta-5,7-dien-3-ol]	55 0.033	0.022	15.040	0.459	85	57	85	57	81	83 duplicate
9751	121 [657; Erythritol (4TMS)]	99 [662; Ribose-5-phosphate methoxymine (BP) (5TMS)]	33 0.015	-0.064	10.779	0.313	86	56	92	50	29	139 original
19005	121 [657; Erythritol (4TMS)]	93 [607; Putrescine (4TMS)]	38 0.010	0.412	7.048	0.513	87	55	65	77	9	67 duplicate
18738	121 [657; Erythritol (4TMS)]	47 [NA]	51 -0.021	-0.054	11.201	0.344	88	54	90	52	32	134 duplicate
15422	121 [657; Erythritol (4TMS)]	130 Trehalose	55 -0.036	-0.151	16.666	0.486	89	53	89	43	72	78 duplicate
9742	121 [657; Erythritol (4TMS)]	84 Mannitol	54 -0.038	-0.040	36.617	0.396	90	52	89	53	126	120 original
18270	121 [657; Erythritol (4TMS)]	58 [1TMS]	53 -0.048	-0.057	39.300	0.427	91	51	91	51	130	104 duplicate
		[638; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane]										
16463	121 [657; Erythritol (4TMS)]	36 [596; N-Acetylglutamic acid (2TMS)]	55 -0.057	-0.021	23.634	0.383	92	50	87	55	98	125 duplicate
14333	121 [657; Erythritol (4TMS)]	107 9-(Z)-Octadecenoic acid	55 -0.077	-0.034	35.322	0.410	93	49	88	54	122	111 duplicate
19305	121 [657; Erythritol (4TMS)]	75 Lysine	55 -0.084	-0.178	22.499	0.405	94	48	100	42	95	115 duplicate
17721	121 [657; Erythritol (4TMS)]	4 Phosphoric acid	55 -0.096	-0.070	45.755	0.385	95	47	93	49	138	129 duplicate
10477	121 [657; Erythritol (4TMS)]	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	43 -0.096	-0.112	38.621	0.283	96	46	96	46	129	141 duplicate
18591	121 [657; Erythritol (4TMS)]	67 Citric acid	55 -0.100	-0.129	15.141	0.406	97	45	97	45	62	114 duplicate
17165	121 [657; Erythritol (4TMS)]	70 Glycerol-3-phosphate	55 -0.110	-0.099	31.118	0.352	98	44	95	47	117	132 duplicate
16628	121 [657; Erythritol (4TMS)]	6 Threonine	55 -0.126	-0.091	28.706	0.429	99	43	94	48	115	103 duplicate
10882	121 [657; Erythritol (4TMS)]	72 [918; D-Xylopyranose (4TMS)]	55 -0.142	-0.138	37.096	0.324	100	42	98	44	127	136 duplicate
17520	121 [657; Erythritol (4TMS)]	53 Glycerol-2-phosphate	54 -0.145	-0.222	12.355	0.438	101	41	104	38	46	102 duplicate
15965	121 [657; Erythritol (4TMS)]	68 Glyceric acid-3-phosphate	55 -0.146	-0.224	9.040	0.369	102	40	105	37	20	128 duplicate
17091	121 [657; Erythritol (4TMS)]	108 Octadecenoic acid	55 -0.157	-0.194	11.580	0.442	103	39	101	41	37	99 duplicate
19338	121 [657; Erythritol (4TMS)]	37 Phenylalanine	55 -0.235	-0.312	12.054	0.412	104	38	108	34	44	109 duplicate
14437	121 [657; Erythritol (4TMS)]	2 Serine	55 -0.279	-0.309	30.208	0.391	105	37	107	35	116	121 duplicate
10202	121 [657; Erythritol (4TMS)]	31 [622; Parabenic acid (2TMS)]	53 -0.292	-0.228	25.509	0.381	106	36	106	36	105	127 duplicate
13788	121 [657; Erythritol (4TMS)]	9 Proline	55 -0.296	-0.410	11.002	0.455	107	35	112	30	31	94 duplicate
11147	121 [657; Erythritol (4TMS)]		54 -0.297	-0.217	33.621	0.342	108	34	103	39	121	135 duplicate

10340	121 [657; Erythritol (4TMS)]	3 Ethanolamine	53 -0.289	-0.441	11,776	0.518	109	33	113	29	39	64 duplicate
15877	121 [657; Erythritol (4TMS)]	52 [NA]	38 -0.331	-0.616	15,356	0.542	110	32	122	20	65	45 duplicate
16545	121 [657; Erythritol (4TMS)]	Ornithine; Arginine	55 -0.349	-0.347	46,847	0.383	111	31	109	33	139	126 duplicate
1213352	121 [657; Erythritol (4TMS)]	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	59 -0.355	-0.683	18,207	0.479	112	30	128	18	80	82 duplicate
10063	121 [657; Erythritol (4TMS)]	1 [938; Sulfuric acid (2TMS)]	35 -0.371	-0.459	10,919	0.534	113	29	115	27	30	51 duplicate
18096	121 [657; Erythritol (4TMS)]	81 Tyrosine	55 -0.374	-0.444	39,499	0.607	114	28	114	28	134	15 duplicate
17850	121 [657; Erythritol (4TMS)]	[826; beta-[[[5-methyl-2-thienyl)methyl]eneamino- benzeneacetic acid methyl ester]	53 -0.380	-0.405	35,449	0.389	115	27	111	31	123	123 duplicate
111015	121 [657; Erythritol (4TMS)]	8 Isoleucine	46 -0.401	-0.214	24,874	0.312	116	28	102	40	102	140 duplicate
141422	121 [657; Erythritol (4TMS)]	34 Aspartic acid	55 -0.409	-0.477	39,438	0.406	117	25	116	26	133	113 duplicate
12890	121 [657; Erythritol (4TMS)]	23 Homoserine	55 -0.414	-0.690	18,529	0.488	118	24	129	13	83	77 duplicate
16706	121 [657; Erythritol (4TMS)]	61 [NA]	55 -0.418	-0.400	13,904	0.448	119	23	110	32	58	98 duplicate
13907	121 [657; Erythritol (4TMS)]	32 [729; N,N-Dimethyllysine methyl ester]	54 -0.419	-0.529	17,518	0.482	120	22	119	23	77	80 duplicate
15515	121 [657; Erythritol (4TMS)]	48 Asparagine	55 -0.440	-0.698	17,998	0.538	121	21	130	12	78	50 duplicate
18830	121 [657; Erythritol (4TMS)]	45 [770; 3,4,6-Trisubhydroxyphenylethanolamine (5TMS)]	41 -0.459	-0.678	11,558	0.472	122	20	125	17	36	88 duplicate
15040	121 [657; Erythritol (4TMS)]	93 [548; Leucine (2TBS)]	51 -0.465	-0.598	16,435	0.418	123	19	121	21	70	108 duplicate
11278	121 [657; Erythritol (4TMS)]	10 Glycine	55 -0.465	-0.732	26,602	0.594	124	18	133	9	109	21 duplicate
16863	121 [657; Erythritol (4TMS)]	63 Glutamine	44 -0.467	-0.650	16,707	0.578	125	17	123	19	73	31 duplicate
13698	121 [657; Erythritol (4TMS)]	30 [815; Ethyl-3-(2H)-thiophenone]	55 -0.472	-0.482	36,578	0.361	126	16	117	25	125	130 duplicate
14075	121 [657; Erythritol (4TMS)]	33 Methionine	55 -0.481	-0.588	18,365	0.420	127	15	120	22	82	107 duplicate
18963	121 [657; Erythritol (4TMS)]	98 [697; Ribose-5-phosphate methoxoyamine (5TMS)]	40 -0.495	-0.725	13,031	0.504	128	14	132	10	52	71 duplicate
14942	121 [657; Erythritol (4TMS)]	42 Glutamic acid	51 -0.508	-0.507	35,497	0.350	129	13	118	24	124	133 duplicate
17310	121 [657; Erythritol (4TMS)]	69 Arginine	51 -0.520	-0.710	28,368	0.513	130	12	131	11	114	68 duplicate
15233	121 [657; Erythritol (4TMS)]	45 Homocysteine	52 -0.549	-0.735	13,332	0.452	131	11	134	8	54	96 duplicate
131213	121 [657; Erythritol (4TMS)]	25 [709; 2,5-Diaminovalerolactam (2TMS)]	44 -0.552	-0.685	16,196	0.529	132	10	127	15	67	52 duplicate
9743	121 [657; Erythritol (4TMS)]	131 [626; 5-Methylthiadenosine (3TMS)]	47 -0.563	-0.757	11,507	0.524	133	9	136	6	35	59 original
12533	121 [657; Erythritol (4TMS)]	20 [619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	22 -0.576	-0.829	12,600	0.576	134	8	138	4	48	32 duplicate
18540	121 [657; Erythritol (4TMS)]	89 [775; Dopamine (4TMS)]	28 -0.577	-0.787	16,567	0.506	135	7	137	5	71	70 duplicate
15198	121 [657; Erythritol (4TMS)]	55 [612; 4-Aminobutyric acid (2TBS)]	34 -0.579	-0.674	15,675	0.475	136	6	128	18	68	84 duplicate
16738	121 [657; Erythritol (4TMS)]	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	35 -0.593	-0.687	12,696	0.477	137	5	124	14	50	86 duplicate
15607	121 [657; Erythritol (4TMS)]	49 [877; Pyrophosphoric acid (4TMS)]	55 -0.616	-0.747	18,017	0.523	138	4	135	7	79	61 duplicate
181815	121 [657; Erythritol (4TMS)]	82 Lysine	31 -0.677	-0.914	22,104	0.570	139	3	141	1	83	34 duplicate
17238	121 [657; Erythritol (4TMS)]	68 [570; Hypoxanthine (2TMS)]	15 -0.733	-0.888	9,980	0.478	140	2	140	2	24	83 duplicate
10613	121 [657; Erythritol (4TMS)]	5 Leucine	36 -0.740	-0.885	15,335	0.502	141	1	139	3	64	73 duplicate
19402	122 [644; Erythritol (4TMS)]	110 [715; Erythritol (4TMS)]	49 0.900	0.974	7,325	0.716	1	141	1	141	8	2 duplicate
18272	122 [644; Erythritol (4TMS)]	106 [733; Threitol (4TMS)]	50 0.889	0.965	15,677	0.728	2	140	3	139	59	1 duplicate
19591	122 [644; Erythritol (4TMS)]	117 [724; Glycerol (3TMS)]	48 0.883	0.971	9,182	0.695	3	139	2	140	14	3 duplicate
18877	122 [644; Erythritol (4TMS)]	121 [657; Erythritol (4TMS)]	48 0.876	0.933	4,516	0.632	4	138	5	137	2	10 duplicate
15138	122 [644; Erythritol (4TMS)]	44 [910; 2-Ketogluconic acid methoxoyamine (4TMS)]	48 0.842	0.961	12,069	0.642	5	137	4	138	28	5 duplicate
9757	122 [644; Erythritol (4TMS)]	126 [559; Erythritol (4TMS)]	45 0.810	0.930	5,943	0.677	6	136	6	136	3	4 original
17767	122 [644; Erythritol (4TMS)]	78 Fructose	52 0.772	0.884	33,774	0.605	7	135	9	133	120	27 duplicate
14744	122 [644; Erythritol (4TMS)]	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	52 0.730	0.904	41,124	0.616	8	134	7	135	135	19 duplicate
19542	122 [644; Erythritol (4TMS)]	115 Glucose-6-phosphate	50 0.657	0.826	32,585	0.630	9	133	21	121	119	12 duplicate
14228	122 [644; Erythritol (4TMS)]	35 Pyrogutamic acid	52 0.627	0.799	48,152	0.557	10	132	27	115	140	52 duplicate
17814	122 [644; Erythritol (4TMS)]	78 Mannose	50 0.618	0.818	11,000	0.582	11	131	22	120	21	35 duplicate
13488	122 [644; Erythritol (4TMS)]	28 Malic acid	52 0.599	0.898	18,064	0.574	12	130	8	134	72	38 duplicate
19047	122 [644; Erythritol (4TMS)]	100 [857; Mannitol (6TMS)]	52 0.597	0.775	17,454	0.559	13	129	33	109	70	49 duplicate
17656	122 [644; Erythritol (4TMS)]	74 [912; Tetradecanoic acid (1TMS)]	45 0.575	0.790	11,706	0.522	14	128	30	112	24	75 duplicate
17589	122 [644; Erythritol (4TMS)]	73 [708; Glucose methoxoyamine (5TMS)]	45 0.572	0.767	11,827	0.520	15	127	31	111	25	78 duplicate
11793	122 [644; Erythritol (4TMS)]	14 Fumaric acid	52 0.534	0.852	10,079	0.564	16	126	13	129	18	43 duplicate

14541	122 [644; Erythritol (4TMS)]	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	52	0.529	0.875	16,094	0.613	17	125	11	131	64	20 duplicate
19126	122 [644; Erythritol (4TMS)]	102	[904; Galactose methoxyamine (5TMS)]	52	0.528	0.706	12,285	0.556	18	124	40	102	30	53 duplicate
12773	122 [644; Erythritol (4TMS)]	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	45	0.523	0.848	6,349	0.604	19	123	15	127	5	28 duplicate
18382	122 [644; Erythritol (4TMS)]	86	[793; D-Galactono-1,4-lactone (4TMS)]	49	0.522	0.849	26,899	0.641	20	122	14	128	106	6 duplicate
13239	122 [644; Erythritol (4TMS)]	26	Citramelic acid	52	0.501	0.766	24,956	0.575	21	121	36	108	99	37 duplicate
14843	122 [644; Erythritol (4TMS)]	39	[929; 1-Phenylethanol (1TMS)]	52	0.488	0.876	22,346	0.608	22	120	10	132	92	23 duplicate
12654	122 [644; Erythritol (4TMS)]	31	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.466	0.890	25,008	0.523	23	119	42	100	100	74 duplicate
		135												
9766	122 [644; Erythritol (4TMS)]		[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	52	0.465	0.655	21,130	0.521	24	118	45	97	90	77 original
16297	122 [644; Erythritol (4TMS)]	56	[929; Orotic acid (3TMS)]	52	0.449	0.827	12,137	0.617	25	117	20	122	27	18 duplicate
15699	122 [644; Erythritol (4TMS)]	50	[746; Ribonic acid-1,4-lactone (3TMS)]	52	0.448	0.806	8,311	0.562	26	115	25	117	10	48 duplicate
16786	122 [644; Erythritol (4TMS)]	62	[812; D-Xylofuranose (4TMS)]	52	0.448	0.780	22,989	0.606	27	116	32	110	95	24 duplicate
19461	122 [644; Erythritol (4TMS)]	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	51	0.443	0.664	10,027	0.524	29	113	43	99	17	73 duplicate
17382	122 [644; Erythritol (4TMS)]	70	[893; 2-Furan-2-hydroxyacetic acid (2TMS)]	45	0.442	0.434	26,891	0.534	30	112	66	76	105	66 duplicate
9763	122 [644; Erythritol (4TMS)]	132	[895; Isomaltose methoxyamine (8TMS)]	40	0.433	0.840	5,981	0.563	31	111	17	125	4	45 original
13578	122 [644; Erythritol (4TMS)]	29	Erythritol	52	0.433	0.780	13,688	0.599	32	110	28	113	41	30 duplicate
17017	122 [644; Erythritol (4TMS)]	65	[646; 3-Deoxyglucitol (5TMS)]	52	0.427	0.856	12,874	0.609	33	108	12	130	34	22 duplicate
13008	122 [644; Erythritol (4TMS)]	24	[725; 2-Ketocanoic acid (2TMS)]	52	0.427	0.839	38,554	0.628	34	109	18	124	133	14 duplicate
9765	122 [644; Erythritol (4TMS)]	134	Isomaltose	52	0.416	0.843	32,509	0.640	35	107	16	126	118	7 original
12044	122 [644; Erythritol (4TMS)]	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	52	0.413	0.809	26,196	0.606	36	106	24	118	103	25 duplicate
18327	122 [644; Erythritol (4TMS)]	85	[529; Methylcitric acid (4TMS)]	36	0.413	0.759	13,314	0.528	37	105	35	107	37	71 duplicate
18489	122 [644; Erythritol (4TMS)]	88	Gluconic acid	52	0.412	0.708	18,592	0.605	38	104	39	103	78	26 duplicate
15329	122 [644; Erythritol (4TMS)]	46	Arabinose	52	0.410	0.828	23,367	0.609	39	103	19	123	97	21 duplicate
19201	122 [644; Erythritol (4TMS)]	104	[795; Erythritol (4TMS)]	51	0.410	0.574	14,873	0.549	40	102	57	85	63	58 duplicate
12291	122 [644; Erythritol (4TMS)]	18	[590; 1-Acetyl-2-thiohydantoin]	52	0.409	0.565	16,775	0.511	41	101	59	83	67	82 duplicate
9771	122 [644; Erythritol (4TMS)]	140	[892; Ergosta-7,22-dien-3-ol (1TMS)]	37	0.405	0.561	9,347	0.418	42	100	60	82	16	114 original
19489	122 [644; Erythritol (4TMS)]	113	Galactose-6-phosphate	50	0.404	0.642	12,232	0.628	43	99	47	95	28	13 duplicate
11666	122 [644; Erythritol (4TMS)]	13	Uracil	52	0.403	0.818	24,220	0.624	44	98	23	119	98	16 duplicate
19657	122 [644; Erythritol (4TMS)]	120	[945; Uridine (3TMS)]	48	0.399	0.240	20,438	0.569	45	97	75	87	81	41 duplicate
11409	122 [644; Erythritol (4TMS)]	11	Succinic acid	52	0.397	0.723	18,988	0.532	46	96	38	104	68	67 duplicate
9772	122 [644; Erythritol (4TMS)]	141	Lanosta-8,24-dien-3-beta-ol	49	0.396	0.568	8,828	0.486	47	95	58	84	12	92 original
11538	122 [644; Erythritol (4TMS)]	12	Glyceric acid	52	0.395	0.765	9,124	0.560	48	94	34	108	13	48 duplicate
		128	[640; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc											
9760	122 [644; Erythritol (4TMS)]			51	0.395	0.803	14,103	0.603	49	93	26	116	45	29 original
19516	122 [644; Erythritol (4TMS)]	114	Fructose-6-phosphate	43	0.382	0.636	9,299	0.622	50	92	50	92	15	17 duplicate
18786	122 [644; Erythritol (4TMS)]	94	Hexadecanoic acid	52	0.380	0.647	27,911	0.550	51	91	46	96	111	57 duplicate
19371	122 [644; Erythritol (4TMS)]	109	Octadecanoic acid	52	0.373	0.693	27,814	0.543	52	90	41	101	110	61 duplicate
9758	122 [644; Erythritol (4TMS)]	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.371	0.605	8,068	0.530	53	89	52	90	9	69 original
9759	122 [644; Erythritol (4TMS)]	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	44	0.368	0.657	13,037	0.538	54	88	44	98	35	64 original
9756	122 [644; Erythritol (4TMS)]	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru	52	0.365	0.576	40,678	0.518	55	87	58	86	134	80 original
12413	122 [644; Erythritol (4TMS)]	19	Alanine (BP) (3TMS)	52	0.356	0.803	20,886	0.564	56	86	53	89	85	44 duplicate
14844	122 [644; Erythritol (4TMS)]	41	[639; Proline (2TMS)]	52	0.348	0.519	22,506	0.498	57	85	63	79	93	87 duplicate
		122	[644; Erythritol (4TMS)]											
16381	122 [644; Erythritol (4TMS)]			49	0.342	0.791	17,343	0.635	58	84	28	114	69	8 duplicate
12168	122 [644; Erythritol (4TMS)]	17	[700; 2-methyl-1,2-propanediol (2TMS)]	52	0.329	0.736	26,129	0.543	59	83	37	105	102	60 duplicate
19164	122 [644; Erythritol (4TMS)]	103	[648; Ethylamine (2TMS)]	52	0.321	0.548	20,071	0.507	60	82	61	81	79	84 duplicate
19373	122 [644; Erythritol (4TMS)]	105	[705; 2-Ketogluconic acid (5TMS)]	48	0.303	0.593	15,950	0.530	61	81	55	87	63	70 duplicate
18891	122 [644; Erythritol (4TMS)]	92	[680; Glycerol-2-phosphate (4TMS)]	49	0.301	0.508	13,416	0.524	62	80	64	78	38	72 duplicate
19636	122 [644; Erythritol (4TMS)]	119	[931; myo-Inositol-2-phosphate (7TMS)]	52	0.282	0.411	14,499	0.455	63	79	67	75	48	102 duplicate
9769	122 [644; Erythritol (4TMS)]	138	[674; Ergosterol (1TMS)]	36	0.273	0.402	10,111	0.471	64	78	68	74	19	99 original
18214	122 [644; Erythritol (4TMS)]	83	Sorbitol	46	0.264	0.007	28,446	0.391	65	77	80	52	112	127 duplicate

9768	122 [644; Erythritol (4TMS)]	137 Ergosterol	52 0.261	0.204	21.043	0.415	68	76	79	63	88	115 original
9754	122 [644; Erythritol (4TMS)]	123 [945; Galactofuranose-6-phosphate (7TMS)]	52 0.255	0.384	20.401	0.554	67	75	70	72	80	55 original
10749	122 [644; Erythritol (4TMS)]	5 Glycerol	52 0.252	0.449	48.580	0.554	68	74	65	77	141	54 duplicate
16053	122 [644; Erythritol (4TMS)]	6 [NA]	49 0.252	0.639	8.738	0.561	69	73	48	94	11	47 duplicate
19087	122 [644; Erythritol (4TMS)]	101 [832; Dopamine (4TMS)]	52 0.225	0.363	18.203	0.401	70	72	72	70	74	123 duplicate
9764	122 [644; Erythritol (4TMS)]	133 [855; Squalene]	52 0.219	0.227	15.864	0.412	71	71	78	64	61	120 original
19432	122 [644; Erythritol (4TMS)]	111 [583; Erythritol (4TMS)]	38 0.215	0.286	13.462	0.435	72	70	73	69	39	107 duplicate
18436	122 [644; Erythritol (4TMS)]	87 [945; beta-D-Glucopyranose (5TMS)]	50 0.200	0.540	43.075	0.540	73	69	62	80	136	63 duplicate
18921	122 [644; Erythritol (4TMS)]	97 [756; beta-D-Methylglucopyranoside (4TMS)]	50 0.193	0.395	27.510	0.517	74	68	69	73	108	81 duplicate
		124 [734; 1-Monooleoylglycerol (2TMS); 1-Monoheptadecanoylglycerol (1TMS)]										
9755	122 [644; Erythritol (4TMS)]	71 [731; Erythritol (4TMS)]	47 0.169	0.137	14.932	0.448	75	67	85	57	54	104 original
17452	122 [644; Erythritol (4TMS)]	96 myo-Inositol	37 0.132	0.124	12.283	0.316	-77	65	86	56	29	140 duplicate
18877	122 [644; Erythritol (4TMS)]	116 [882; Pseudouridine (5TMS)]	22 0.126	0.598	6.980	0.558	78	64	54	88	7	50 duplicate
19567	122 [644; Erythritol (4TMS)]	91 [766; beta-D-Methylglucopyranoside (4TMS)]	52 0.097	0.236	23.242	0.429	79	62	76	66	96	109 duplicate
18642	122 [644; Erythritol (4TMS)]	107 [9-Z]-Octadecenoic acid	52 0.084	0.183	15.799	0.399	81	61	80	62	60	124 duplicate
19306	122 [644; Erythritol (4TMS)]	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	30 0.057	0.148	12.581	0.356	83	59	84	58	32	137 duplicate
18592	122 [644; Erythritol (4TMS)]	139 [700; Ergosta-5,7-dien-3-ol]	50 0.048	0.371	39.229	0.480	84	58	71	71	131	96 duplicate
9770	122 [644; Erythritol (4TMS)]	83 [607; Putrescine (4TMS)]	38 0.021	0.636	6.566	0.634	85	57	49	93	6	9 duplicate
18037	122 [644; Erythritol (4TMS)]	90 [772; D-Glucose (5TMS)]	17 0.015	0.173	3.665	0.472	86	56	81	61	1	98 original
19006	122 [644; Erythritol (4TMS)]	99 [662; Ribose-5-phosphate methoxamine (BP) (5TMS)]	50 0.011	0.167	38.680	0.542	87	55	82	60	130	62 duplicate
9767	122 [644; Erythritol (4TMS)]	138 [748; D-Sedoheptulose-7-phosphate (7TMS)]	52 -0.002	0.265	43.189	0.565	88	54	74	68	137	34 duplicate
18271	122 [644; Erythritol (4TMS)]	84 Mannitol	52 -0.008	0.008	11.391	0.349	89	53	89	53	22	139 duplicate
17976	122 [644; Erythritol (4TMS)]	53 Glycerol-2-phosphate	52 -0.023	-0.097	31.227	0.425	90	52	93	49	117	111 duplicate
15966	122 [644; Erythritol (4TMS)]	67 Citric acid	52 -0.036	-0.142	37.130	0.497	91	51	95	47	126	89 original
17166	122 [644; Erythritol (4TMS)]	130 Trehalose	52 -0.038	-0.052	18.170	0.573	92	50	92	50	73	39 duplicate
9761	122 [644; Erythritol (4TMS)]	47 [NA]	52 -0.042	-0.199	35.608	0.458	93	49	88	44	123	101 duplicate
15423	122 [644; Erythritol (4TMS)]	36 [596; N-Acetylglutamic acid (2TMS)]	49 -0.061	-0.047	13.874	0.425	94	48	91	51	44	112 duplicate
14334	122 [644; Erythritol (4TMS)]	118 [928; Glucopyranose-6-phosphate (6TMS)]	52 -0.094	-0.180	14.819	0.411	95	47	97	45	52	121 duplicate
19614	122 [644; Erythritol (4TMS)]	84 [789; Tyramine (3TMS)]	34 -0.098	-0.361	15.885	0.581	96	46	106	38	62	38 duplicate
15978	122 [644; Erythritol (4TMS)]	52 [NA]	52 -0.107	-0.131	28.969	0.472	97	45	94	48	115	97 duplicate
16627	122 [644; Erythritol (4TMS)]	60 Glycerol-3-phosphate	39 -0.155	-0.244	38.295	0.380	98	44	101	41	128	132 duplicate
10478	122 [644; Erythritol (4TMS)]	4 Phosphoric acid										
		[636; 4R-Acetylido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]										
16464	122 [644; Erythritol (4TMS)]	58 [1TMS]	52 -0.163	-0.219	25.281	0.454	99	43	100	42	101	103 duplicate
17521	122 [644; Erythritol (4TMS)]	72 [918; D-Xylopyranose (4TMS)]	51 -0.181	-0.157	14.765	0.380	100	42	98	46	51	131 duplicate
17092	122 [644; Erythritol (4TMS)]	66 Glycic acid-3-phosphate	52 -0.196	-0.378	14.461	0.510	101	41	110	32	47	83 duplicate
11919	122 [644; Erythritol (4TMS)]	15 Alanine	52 -0.198	-0.218	28.896	0.551	102	40	99	43	113	56 duplicate
19339	122 [644; Erythritol (4TMS)]	108 Octadecenoic acid	52 -0.216	-0.320	14.240	0.420	103	39	105	37	46	113 duplicate
17722	122 [644; Erythritol (4TMS)]	75 Lysine	52 -0.217	-0.297	45.760	0.492	104	38	103	39	138	90 duplicate
10341	122 [644; Erythritol (4TMS)]	3 Ethanolamine	50 -0.220	-0.445	13.862	0.498	105	37	114	28	43	88 duplicate
10883	122 [644; Erythritol (4TMS)]	7 Threonine	52 -0.226	-0.294	37.260	0.362	106	36	102	40	127	135 duplicate
16864	122 [644; Erythritol (4TMS)]	63 Glutamine	40 -0.244	-0.428	15.319	0.573	107	35	112	30	55	40 duplicate
14438	122 [644; Erythritol (4TMS)]	37 Phenylalanine	52 -0.253	-0.392	30.573	0.412	108	34	111	31	116	119 duplicate
10064	122 [644; Erythritol (4TMS)]	1 [938; Sulfuric acid (2TMS)]	36 -0.254	0.022	10.280	0.631	109	33	88	54	20	11 duplicate
18832	122 [644; Erythritol (4TMS)]	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	38 -0.314	-0.542	12.787	0.413	110	32	118	24	33	116 duplicate
10203	122 [644; Erythritol (4TMS)]	2 Serine	50 -0.334	-0.377	27.373	0.413	111	31	109	33	108	118 duplicate
13799	122 [644; Erythritol (4TMS)]	31 [622; Parabanic acid (2TMS)]	52 -0.341	-0.582	14.578	0.485	112	30	120	22	49	93 duplicate
		[826; beta-[[[5-methyl-2-thienyl)methyl]ensaminio-benzeneacetic acid methyl ester]										
17851	122 [644; Erythritol (4TMS)]	77 benzeneacetic acid methyl ester]	50 -0.349	-0.475	34.993	0.398	113	29	115	27	122	125 duplicate

16097	122	[644; Erythritol (4TMS)]	81	Tyrosine	52	-0.354	-0.519	38,453	0.627	114	28	116	26	129	15 duplicate
11148	122	[644; Erythritol (4TMS)]	9	Proline	51	-0.357	-0.364	34,510	0.392	115	27	107	35	121	128 duplicate
16546	122	[644; Erythritol (4TMS)]	59	Ornithine; Arginine	52	-0.359	-0.442	46,259	0.429	116	26	113	29	139	110 duplicate
16707	122	[644; Erythritol (4TMS)]	61	[NA]	52	-0.367	-0.371	15,647	0.434	117	25	108	34	58	108 duplicate
13353	122	[644; Erythritol (4TMS)]	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	41	-0.368	-0.780	21,307	0.499	118	24	132	10	91	86 duplicate
15516	122	[644; Erythritol (4TMS)]	48	Asparagine	52	-0.418	-0.729	19,255	0.557	119	23	130	12	77	51 duplicate
13908	122	[644; Erythritol (4TMS)]	32	[729; N,N-Dimethyllysine methyl ester]	51	-0.424	-0.657	20,893	0.547	120	22	125	17	86	59 duplicate
111016	122	[644; Erythritol (4TMS)]	8	Isoleucine	43	-0.435	-0.317	26,522	0.358	121	21	104	38	104	138 duplicate
12891	122	[644; Erythritol (4TMS)]	23	Homoserine	52	-0.440	-0.797	20,951	0.532	122	20	133	9	87	68 duplicate
111279	122	[644; Erythritol (4TMS)]	10	Glycine	52	-0.449	-0.828	27,037	0.596	123	19	137	5	107	32 duplicate
14123	122	[644; Erythritol (4TMS)]	34	Aspartic acid	52	-0.462	-0.539	39,540	0.389	124	18	117	25	132	128 duplicate
18541	122	[644; Erythritol (4TMS)]	89	[775; Dopamine (4TMS)]	23	-0.470	-0.725	16,256	0.488	125	17	128	14	65	91 duplicate
15041	122	[644; Erythritol (4TMS)]	43	[548; Leucine (2TBS)]	48	-0.496	-0.620	18,702	0.369	126	16	123	19	75	134 duplicate
13689	122	[644; Erythritol (4TMS)]	30	[815; Ethyl-3(2H)-thiophenone]	52	-0.501	-0.560	36,841	0.353	127	15	119	23	125	138 duplicate
14016	122	[644; Erythritol (4TMS)]	33	Methionine	48	-0.520	-0.643	20,490	0.388	128	14	124	18	82	130 duplicate
14943	122	[644; Erythritol (4TMS)]	42	Glutamic acid	48	-0.521	-0.608	35,861	0.389	129	13	121	21	124	129 duplicate
15234	122	[644; Erythritol (4TMS)]	45	Homocysteine	49	-0.529	-0.689	15,600	0.447	130	12	127	15	57	105 duplicate
17311	122	[644; Erythritol (4TMS)]	69	Arginine	48	-0.553	-0.798	28,938	0.566	131	11	134	8	114	42 duplicate
9762	122	[644; Erythritol (4TMS)]	131	[626; 5-Methylthiadenosine (3TMS)]	44	-0.556	-0.729	13,759	0.506	132	10	129	13	42	85 original
18904	122	[644; Erythritol (4TMS)]	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	37	-0.559	-0.827	15,531	0.483	133	9	136	6	56	95 duplicate
15789	122	[644; Erythritol (4TMS)]	51	[489; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	32	-0.560	-0.752	14,718	0.413	134	8	131	11	50	117 duplicate
15608	122	[644; Erythritol (4TMS)]	49	[877; Pyrophosphoric acid (4TMS)]	52	-0.587	-0.657	18,922	0.520	135	7	126	16	79	79 duplicate
161139	122	[644; Erythritol (4TMS)]	55	[612; 4-Aminobutyric acid (2TBS)]	31	-0.587	-0.618	16,283	0.463	136	6	122	20	68	100 duplicate
13124	122	[644; Erythritol (4TMS)]	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.592	-0.863	20,718	0.586	137	5	138	4	84	33 duplicate
17239	122	[644; Erythritol (4TMS)]	68	[570; Hypoxanthine (2TMS)]	11	-0.600	-0.908	11,550	0.288	138	4	140	2	23	141 duplicate
12534	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	19	-0.696	-0.826	13,171	0.535	139	3	135	7	36			65 duplicate
10614	122	[644; Erythritol (4TMS)]	5	Leucine	33	-0.720	-0.887	17,881	0.522	140	2	139	3	71	76 duplicate
18156	122	[644; Erythritol (4TMS)]	82	Lysine	27	-0.744	-0.929	20,814	0.599	141	1	141	1	83	31 duplicate
19517	123	[945; Galactofuranose-6	114	Fructose-6-phosphate	53	0.801	0.914	11,441	0.659	1	141	1	141	42	2 duplicate
19490	123	[945; Galactofuranose-6	113	Galactose-6-phosphate	62	0.722	0.854	11,603	0.643	2	140	3	139	44	4 duplicate
12414	123	[945; Galactofuranose-6	19	Alanine (BP) (3TMS)	64	0.823	0.850	3,748	0.603	3	139	4	138	1	13 duplicate
17877	123	[945; Galactofuranose-6	79	Glucose	64	0.601	0.861	25,623	0.596	4	138	2	140	129	14 duplicate
19202	123	[945; Galactofuranose-6	104	[795; Erythritol (4TMS)]	63	0.554	0.735	8,135	0.568	5	137	11	131	17	24 duplicate
14845	123	[945; Galactofuranose-6	41	[639; Proline (2TMS)]	64	0.547	0.744	4,591	0.561	6	136	10	132	5	28 duplicate
11920	123	[945; Galactofuranose-6	15	Alanine	64	0.533	0.790	9,054	0.572	7	135	5	137	28	22 duplicate
19543	123	[945; Galactofuranose-6	115	Glucose-6-phosphate	62	0.528	0.782	15,520	0.520	8	134	6	136	77	52 duplicate
17590	123	[945; Galactofuranose-6	73	[708; Glucose methoxyamine (5TMS)]	57	0.521	0.712	12,748	0.521	9	133	12	130	53	51 duplicate
14230	123	[945; Galactofuranose-6	35	Pyroglutamic acid	64	0.503	0.760	32,308	0.543	10	132	7	135	139	39 duplicate
16942	123	[945; Galactofuranose-6	83	Sorbitol	63	0.491	0.683	8,887	0.418	11	131	15	127	26	122 duplicate
18215	123	[945; Galactofuranose-6	83	[4TMS]]	58	0.488	0.301	13,021	0.417	12	130	67	75	54	123 duplicate
18273	123	[945; Galactofuranose-6	106	[733; Threitol (4TMS)]	62	0.474	0.702	8,640	0.618	13	129	13	129	22	10 duplicate
19568	123	[945; Galactofuranose-6	116	[882; Pseudouridine (5TMS)]	30	0.444	0.221	11,358	0.501	14	128	75	67	41	62 duplicate
17815	123	[945; Galactofuranose-6	70	Mannose	62	0.439	0.679	13,760	0.493	15	127	16	126	65	66 duplicate
17363	123	[945; Galactofuranose-6	121	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	0.429	0.668	9,886	0.508	16	126	17	125	32	60 duplicate
18678	123	[945; Galactofuranose-6	121	[657; Erythritol (4TMS)]	55	0.415	0.608	18,597	0.492	17	125	21	121	83	67 duplicate
17768	123	[945; Galactofuranose-6	76	Fructose	64	0.392	0.747	16,725	0.531	18	124	9	133	86	47 duplicate
9785	123	[945; Galactofuranose-6	136	[748; D-Scetoheptulose-7-phosphate (7TMS)]	17	0.382	0.507	5,522	0.467	19	123	32	110	9	87 original
18878	123	[945; Galactofuranose-6	96	myo-Inositol	49	0.381	0.297	23,836	0.345	20	122	68	74	121	141 duplicate
9774	123	[945; Galactofuranose-6	125	[892; Sucrose (6TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	0.377	0.751	22,848	0.522	21	121	8	134	115	50 original
13467	123	[945; Galactofuranose-6	28	Malic acid	64	0.368	0.478	4,202	0.476	22	120	35	107	2	75 duplicate



19088	123 [945; Galactofuranose-6	101	[832; Dopamine (4TMS)]	64	0.128	0.121	11.569	0.504	73	70	82	60	43	61 duplicate
15700	123 [945; Galactofuranose-6	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	0.120	0.311	24.129	0.475	74	68	66	76	123	78 duplicate
18787	123 [945; Galactofuranose-6	94	Hexadecanoic acid	64	0.118	0.448	13.231	0.538	75	67	38	104	59	43 duplicate
9798	123 [945; Galactofuranose-6	139	[700; Ergosta-5,7-dien-3-ol]	38	0.115	-0.009	21.667	0.414	76	68	90	52	108	125 original
19658	123 [945; Galactofuranose-6	120	[945; Uridine (3TMS)]	54	0.113	0.035	6.377	0.434	77	65	88	54	11	107 duplicate
11539	123 [945; Galactofuranose-6	12	Glyceric acid	63	0.110	0.227	16.282	0.389	78	64	74	68	83	135 duplicate
9778	123 [945; Galactofuranose-6	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	0.107	0.410	13.355	0.564	79	63	48	94	61	26 original
18643	123 [945; Galactofuranose-6	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	0.070	0.041	17.622	0.548	80	62	86	56	91	37 duplicate
10204	123 [945; Galactofuranose-6	2	Serine	62	0.067	0.128	14.337	0.450	81	61	81	61	69	98 duplicate
16628	123 [945; Galactofuranose-6	60	Glycerol-3-phosphate	64	0.065	-0.087	13.177	0.540	82	60	94	48	56	41 duplicate
17093	123 [945; Galactofuranose-6	86	Glyceric acid-3-phosphate	64	0.060	0.134	10.955	0.516	83	59	80	62	38	57 duplicate
9776	123 [945; Galactofuranose-6	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.047	-0.076	8.628	0.459	84	58	96	46	21	93 original
10478	123 [945; Galactofuranose-6	4	Phosphoric acid	51	0.040	0.110	24.985	0.421	85	57	84	58	127	118 duplicate
13354	123 [945; Galactofuranose-6	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	0.001	-0.208	22.841	0.419	86	56	110	32	114	119 duplicate
9773	123 [945; Galactofuranose-6	124	[734; 1-Monocoleoylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	59	-0.001	-0.040	28.589	0.394	87	55	91	51	136	132 original
9790	123 [945; Galactofuranose-6	141	Lanosta-8,24-dien-3-beta-ol	61	-0.001	-0.083	19.230	0.417	88	54	97	45	97	124 original
16054	123 [945; Galactofuranose-6	54	[NA]	55	-0.003	0.261	17.023	0.483	89	53	71	71	89	72 duplicate
17167	123 [945; Galactofuranose-6	67	Citric acid	64	-0.004	-0.138	15.201	0.486	90	52	103	39	75	69 duplicate
18692	123 [945; Galactofuranose-6	92	[680; Glycerol-2-phosphate (4TMS)]	54	-0.006	0.443	11.321	0.447	91	51	41	101	39	102 duplicate
14439	123 [945; Galactofuranose-6	37	Phenylalanine	64	-0.011	-0.074	14.244	0.493	92	50	95	47	68	65 duplicate
9786	123 [945; Galactofuranose-6	137	Ergosterol	64	-0.013	-0.005	10.210	0.387	93	49	89	53	35	138 original
16382	123 [945; Galactofuranose-6	57	[757; 2-Deoxy-pentose-3-ylose dimethoxyamine (2TMS)]	55	-0.026	0.369	13.182	0.528	94	48	58	84	57	49 duplicate
11149	123 [945; Galactofuranose-6	9	Proline	63	-0.041	0.090	21.077	0.433	95	47	85	57	105	109 duplicate
18965	123 [945; Galactofuranose-6	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	48	-0.078	-0.256	23.197	0.409	96	46	112	30	117	128 duplicate
13909	123 [945; Galactofuranose-6	32	[728; N-Dimethyllysine methyl ester]	63	-0.078	-0.085	20.008	0.513	97	45	99	43	100	59 duplicate
9777	123 [945; Galactofuranose-6	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	-0.089	-0.133	8.793	0.473	98	44	102	40	24	80 original
13800	123 [945; Galactofuranose-6	31	[622; Parabanic acid (2TMS)]	62	-0.091	-0.117	15.864	0.448	99	43	101	41	78	100 duplicate
10342	123 [945; Galactofuranose-6	3	Ethanolamine	62	-0.104	-0.385	16.539	0.595	100	42	117	25	85	15 duplicate
18098	123 [945; Galactofuranose-6	81	Tyrosine	64	-0.106	-0.309	26.581	0.652	101	41	115	27	133	3 duplicate
16547	123 [945; Galactofuranose-6	59	Ornithine; Arginine	64	-0.113	-0.082	32.462	0.432	102	40	93	49	140	110 duplicate
17522	123 [945; Galactofuranose-6	72	[919; D-Xylopyranose (4TMS)]	64	-0.114	-0.185	13.749	0.380	103	39	108	34	64	140 duplicate
12892	123 [945; Galactofuranose-6	23	Homoserine	63	-0.128	-0.195	12.117	0.444	104	38	114	28	49	104 duplicate
15042	123 [945; Galactofuranose-6	43	[548; Leucine (2TBS)]	60	-0.130	-0.186	8.335	0.476	105	37	109	33	18	74 duplicate
17852	123 [945; Galactofuranose-6	77	[826; beta-[[[5-methyl-2-thienyl)methyleneamino-benzeneacetic acid methyl ester]	62	-0.151	-0.171	22.961	0.474	106	36	107	35	116	78 duplicate
15424	123 [945; Galactofuranose-6	47	[NA]	64	-0.173	-0.207	13.280	0.469	107	35	111	31	60	83 duplicate
19007	123 [945; Galactofuranose-6	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	-0.173	0.155	14.377	0.519	108	34	79	63	70	53 duplicate
14124	123 [945; Galactofuranose-6	34	Aspartic acid	64	-0.176	-0.139	24.667	0.390	109	33	104	38	126	134 duplicate
14017	123 [945; Galactofuranose-6	33	Methionine	64	-0.177	-0.168	11.974	0.383	110	32	106	36	47	139 duplicate
11017	123 [945; Galactofuranose-6	8	Isoleucine	55	-0.177	0.038	13.927	0.403	111	31	87	55	67	130 duplicate
13690	123 [945; Galactofuranose-6	30	[815; Ethyl-3(2H)-thiophenone]	64	-0.183	-0.085	22.297	0.396	112	30	98	44	112	131 duplicate
19340	123 [945; Galactofuranose-6	108	Octadecanoic acid	64	-0.188	-0.265	12.286	0.390	113	29	113	29	50	133 duplicate
13125	123 [945; Galactofuranose-6	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.199	-0.087	16.718	0.485	114	28	100	42	94	70 duplicate
18922	123 [945; Galactofuranose-6	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	-0.199	-0.060	17.023	0.625	115	27	92	50	88	9 duplicate
17312	123 [945; Galactofuranose-6	69	Arginine	60	-0.217	-0.346	16.014	0.519	116	26	116	26	80	64 duplicate
14944	123 [945; Galactofuranose-6	42	Glutamic acid	60	-0.231	-0.154	23.598	0.438	117	25	105	37	119	108 duplicate
19307	123 [945; Galactofuranose-6	107	9-(Z)-Octadecenoic acid	64	-0.234	-0.393	7.768	0.453	118	24	119	23	14	95 duplicate
11260	123 [945; Galactofuranose-6	10	Glycine	64	-0.238	-0.488	13.211	0.557	119	23	127	15	58	31 duplicate

19637	123 [945; Galactofuranose-6 119 [931; myo-Inositol-2-phosphate (7TMS)]	64 -0.242	-0.415	9.983	0.471	120	22	121	21	33	81 duplicate
15325	123 [945; Galactofuranose-6 45 Homocysteine	61 -0.289	-0.427	27.043	0.428	121	21	125	17	134	113 duplicate
18593	123 [945; Galactofuranose-6 90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	64 -0.290	-0.445	8.670	0.462	122	20	126	16	23	90 duplicate
19238	123 [945; Galactofuranose-6 105 [705; 2-Ketogluconic acid (5TMS)]	48 -0.312	-0.568	13.037	0.551	123	18	130	12	55	36 duplicate
15967	123 [945; Galactofuranose-6 53 Glycerol-2-phosphate	64 -0.313	-0.388	16.416	0.387	124	18	118	24	84	137 duplicate
15517	123 [945; Galactofuranose-6 48 Asparagine	64 -0.337	-0.628	14.539	0.554	125	17	132	10	72	33 duplicate
15790	123 [945; Galactofuranose-6 51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44 -0.342	-0.418	24.207	0.433	126	16	123	19	124	108 duplicate
18272	123 [945; Galactofuranose-6 84 Mannitol	62 -0.350	-0.417	25.069	0.517	127	15	122	20	128	56 duplicate
18708	123 [945; Galactofuranose-6 61 [NA]	64 -0.357	-0.547	9.491	0.462	128	14	129	13	29	89 duplicate
10065	123 [945; Galactofuranose-6 1 [938; Sulfuric acid (2TMS)]	60 -0.388	-0.397	22.338	0.425	129	13	120	22	113	116 duplicate
9780	123 [945; Galactofuranose-6 93 [607; Putrescine (4TMS)]	36 -0.425	-0.421	11.831	0.610	130	12	124	18	45	12 duplicate
15609	123 [945; Galactofuranose-6 131 [626; 5-Methylthioadenosine (3TMS)]	55 -0.436	-0.690	21.910	0.576	131	11	134	8	110	20 original
18833	123 [945; Galactofuranose-6 49 [877; Pyrophosphoric acid (4TMS)]	64 -0.447	-0.634	26.254	0.428	132	10	133	9	131	112 duplicate
17240	123 [945; Galactofuranose-6 95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50 -0.450	-0.618	23.898	0.498	133	9	131	11	122	63 duplicate
18157	123 [945; Galactofuranose-6 68 [570; Hypoxanthine (2TMS)]	20 -0.474	-0.873	16.131	0.590	134	8	137	5	81	18 duplicate
16140	123 [945; Galactofuranose-6 82 Lysine	39 -0.511	-0.841	15.934	0.660	135	7	136	6	79	1 duplicate
10615	123 [945; Galactofuranose-6 55 [612; 4-Aminobutyric acid (2TBS)]	43 -0.539	-0.907	27.341	0.592	136	6	139	3	135	17 duplicate
12535	123 [945; Galactofuranose-6 5 Leucine	45 -0.552	-0.517	14.829	0.478	137	5	128	14	74	73 duplicate
15979	123 [945; Galactofuranose-6 20 [619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31 -0.591	-0.878	19.080	0.630	138	4	138	4	95	6 duplicate
18665	123 [945; Galactofuranose-6 52 [NA]	46 -0.648	-0.910	23.624	0.638	139	3	140	2	120	5 duplicate
18542	123 [945; Galactofuranose-6 83 Glutamine	52 -0.679	-0.822	20.195	0.534	140	2	135	7	102	45 duplicate
9803	124 [734; 1-Monooligosaccharide 137 Ergosterol	59 0.516	0.913	20.450	0.630	141	1	141	1	104	7 duplicate
18788	124 [734; 1-Monooligosaccharide 94 Hexadecanoic acid	59 0.490	0.511	39.777	0.458	2	140	13	129	115	38 original
9804	124 [734; 1-Monooligosaccharide 141 Lanosta-8,24-dien-3-beta-ol	56 0.486	0.619	11.873	0.459	3	139	1	141	17	11 duplicate
18373	124 [734; 1-Monooligosaccharide 109 Octadecanoic acid	46 0.459	0.590	6.255	0.484	4	138	5	137	7	9 original
19638	124 [734; 1-Monooligosaccharide 119 [931; myo-Inositol-2-phosphate (7TMS)]	59 0.455	0.410	39.761	0.423	5	137	27	115	114	34 duplicate
19308	124 [734; 1-Monooligosaccharide 107 9-(Z)-Octadecenoic acid	59 0.425	0.565	24.483	0.441	6	136	6	136	88	21 duplicate
9782	124 [734; 1-Monooligosaccharide 126 [559; Erythritol (4TMS)]	59 0.407	0.598	32.791	0.464	7	135	3	139	98	7 duplicate
17168	124 [734; 1-Monooligosaccharide 67 Citric acid	40 0.367	0.520	17.836	0.496	8	134	11	131	40	2 original
19569	124 [734; 1-Monooligosaccharide 116 [882; Pseudouridine (5TMS)]	59 0.356	0.448	42.172	0.368	9	133	21	121	117	103 duplicate
18341	124 [734; 1-Monooligosaccharide 108 Octadecanoic acid	30 0.338	0.601	13.340	0.503	10	132	2	140	22	1 duplicate
10343	124 [734; 1-Monooligosaccharide 3 Ethanolamine	59 0.335	0.513	19.078	0.362	11	131	12	130	44	108 duplicate
9806	124 [734; 1-Monooligosaccharide 140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	57 0.328	0.501	15.784	0.387	12	130	14	128	33	79 duplicate
16628	124 [734; 1-Monooligosaccharide 60 Glycerol-3-phosphate	47 0.323	0.449	6.194	0.439	13	129	20	122	6	22 original
18329	124 [734; 1-Monooligosaccharide 85 [529; Methylcitric acid (4TMS)]	59 0.321	0.465	39.744	0.374	14	128	17	125	113	92 duplicate
9799	124 [734; 1-Monooligosaccharide 133 [855; Squalene]	44 0.313	0.328	17.382	0.422	15	127	33	109	38	36 duplicate
18594	124 [734; 1-Monooligosaccharide 90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	59 0.309	0.523	23.031	0.355	16	126	10	132	62	122 original
12536	124 [734; 1-Monooligosaccharide 77 benzeneacetic acid methyl ester]	59 0.305	0.423	24.243	0.417	17	125	24	118	65	44 duplicate
18834	124 [734; 1-Monooligosaccharide 95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	28 0.280	0.304	9.398	0.429	18	124	37	105	16	28 duplicate
17454	124 [734; 1-Monooligosaccharide 71 [731; Erythrose (3TMS)]	45 0.277	0.416	7.331	0.326	19	123	26	116	10	139 duplicate
17853	124 [734; 1-Monooligosaccharide 77 benzeneacetic acid methyl ester]	59 0.275	0.297	30.220	0.384	20	122	38	104	89	83 duplicate
14440	124 [734; 1-Monooligosaccharide 37 Phenylalanine	57 0.268	0.469	48.209	0.358	21	121	16	126	123	115 duplicate
14336	124 [734; 1-Monooligosaccharide 38 [596; N-Acetylglutamic acid (2TMS)]	59 0.264	0.428	41.050	0.376	22	120	23	119	116	81 duplicate
14945	124 [734; 1-Monooligosaccharide 42 Glutamic acid	59 0.262	0.458	48.485	0.367	23	119	19	123	124	104 duplicate
9805	124 [734; 1-Monooligosaccharide 139 [700; Ergosta-5,7-dien-3-ol]	55 0.255	0.437	44.805	0.356	24	118	22	120	122	119 duplicate
18099	124 [734; 1-Monooligosaccharide 81 Tyrosine	38 0.249	0.549	2.905	0.425	25	117	8	134	1	32 original
		59 0.245	0.464	51.494	0.385	26	116	18	124	134	82 duplicate



9786	124 [734; 1-Monoolioleoylglyce 130	Trehalose	58	0.221	0.420	48.008	0.388	27	115	25	117	128	76 original
16548	124 [734; 1-Monoolioleoylglyce 59	Omithine; Arginine	59	0.220	0.276	58.624	0.339	28	114	41	101	139	133 duplicate
19434	124 [734; 1-Monoolioleoylglyce 111	[583; Erythritol (4TMS)]	39	0.206	0.200	3.783	0.380	29	113	48	94	2	87 duplicate
15140	124 [734; 1-Monoolioleoylglyce 44	[910; 2-Ketogluconic acid methoxymamine (4TMS)]	45	0.204	0.139	24.297	0.414	30	112	54	88	67	48 duplicate
10885	124 [734; 1-Monoolioleoylglyce 7	Threonine	59	0.197	0.344	48.297	0.349	31	111	30	112	127	130 duplicate
17658	124 [734; 1-Monoolioleoylglyce 74	[912; Tetradecanoic acid (1TMS)]	59	0.191	0.169	22.036	0.405	32	110	52	90	68	58 duplicate
11281	124 [734; 1-Monoolioleoylglyce 10	Glycine	59	0.172	0.316	36.423	0.404	33	109	35	107	107	57 duplicate
19898	124 [734; 1-Monoolioleoylglyce 122	[644; Erythritol (4TMS)]	47	0.169	0.137	14.932	0.448	34	108	55	87	27	14 duplicate
9788	124 [734; 1-Monoolioleoylglyce 132	[895; Isomaltose methoxymamine (8TMS)]	38	0.169	-0.015	15.083	0.417	35	107	71	71	28	43 original
13910	124 [734; 1-Monoolioleoylglyce 32	[728; N,N-Dimethyllysine methyl ester]	58	0.164	0.371	18.319	0.394	36	108	29	113	42	68 duplicate
15791	124 [734; 1-Monoolioleoylglyce 51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	40	0.154	0.166	7.247	0.371	37	105	53	89	9	98 duplicate
18216	124 [734; 1-Monoolioleoylglyce 83	Sorbitol	53	0.147	0.177	36.911	0.362	38	104	51	91	110	107 duplicate
15880	124 [734; 1-Monoolioleoylglyce 52	[NA]	42	0.141	0.329	12.347	0.359	39	103	32	110	19	114 duplicate
17313	124 [734; 1-Monoolioleoylglyce 69	Arginine	55	0.131	0.291	36.982	0.414	40	102	40	102	111	47 duplicate
13691	124 [734; 1-Monoolioleoylglyce 30	[915; Ethyl-3(2H)-thiophenone]	59	0.126	0.207	47.024	0.352	41	101	46	96	125	123 duplicate
17724	124 [734; 1-Monoolioleoylglyce 75	Lysine	59	0.122	0.333	57.396	0.373	42	100	31	111	138	95 duplicate
11150	124 [734; 1-Monoolioleoylglyce 9	Proline	58	0.122	0.469	42.982	0.368	43	99	15	127	119	101 duplicate
16141	124 [734; 1-Monoolioleoylglyce 55	[912; 4-Aminobutyric acid (2TBS)]	39	0.120	0.324	8.387	0.373	44	98	34	108	11	96 duplicate
11018	124 [734; 1-Monoolioleoylglyce 8	Isoleucine	51	0.107	0.591	32.287	0.356	45	97	4	138	94	120 duplicate
9797	124 [734; 1-Monoolioleoylglyce 131	[826; 5-Methylthiadecosine (3TMS)]	50	0.105	0.116	8.138	0.359	46	96	59	83	13	113 original
19404	124 [734; 1-Monoolioleoylglyce 110	[715; Erythritol (4TMS)]	49	0.102	0.019	20.158	0.447	47	95	67	75	51	15 duplicate
15518	124 [734; 1-Monoolioleoylglyce 48	Asparagine	59	0.099	0.250	24.713	0.396	48	93	44	98	71	64 duplicate
15968	124 [734; 1-Monoolioleoylglyce 53	Glycerol-2-phosphate	59	0.099	0.088	14.362	0.400	49	94	61	81	25	63 duplicate
14018	124 [734; 1-Monoolioleoylglyce 33	Methionine	59	0.081	0.202	24.577	0.363	50	92	47	95	69	106 duplicate
19593	124 [734; 1-Monoolioleoylglyce 117	[724; Glyceral (3TMS)]	51	0.081	0.079	20.983	0.445	51	91	63	79	55	17 duplicate
10205	124 [734; 1-Monoolioleoylglyce 2	Serine	57	0.079	0.532	33.353	0.380	52	90	9	133	97	88 duplicate
16466	124 [734; 1-Monoolioleoylglyce 58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	59	0.079	0.193	33.362	0.352	53	89	49	83	98	124 duplicate
9802	124 [734; 1-Monoolioleoylglyce 136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.074	0.260	11.948	0.457	54	88	43	99	18	12 original
13801	124 [734; 1-Monoolioleoylglyce 31	[822; Parabanic acid (2TMS)]	59	0.073	0.233	15.271	0.346	55	87	45	97	30	131 duplicate
19203	124 [734; 1-Monoolioleoylglyce 104	[785; Erythritol (4TMS)]	58	0.072	0.052	22.508	0.345	56	86	65	77	61	132 duplicate
8794	124 [734; 1-Monoolioleoylglyce 128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	40	0.062	-0.103	23.194	0.480	57	85	81	61	63	5 original
10480	124 [734; 1-Monoolioleoylglyce 4	Phosphoric acid	47	0.049	0.398	48.345	0.356	58	84	28	114	128	118 duplicate
9793	124 [734; 1-Monoolioleoylglyce 127	[777; Fructose-6-phosphate methoxymamine (6TMS)]	35	0.045	0.119	18.388	0.426	59	83	58	84	43	30 original
18049	124 [734; 1-Monoolioleoylglyce 100	[657; Mannitol (6TMS)]	59	0.045	-0.119	26.611	0.391	60	82	84	58	79	73 duplicate
17094	124 [734; 1-Monoolioleoylglyce 66	Glyceric acid-3-phosphate	59	0.044	0.266	19.138	0.351	61	81	42	100	45	127 duplicate
18709	124 [734; 1-Monoolioleoylglyce 61	[NA]	59	0.039	-0.005	22.256	0.362	62	80	70	72	60	110 duplicate
18679	124 [734; 1-Monoolioleoylglyce 121	[657; Erythritol (4TMS)]	50	0.033	0.018	13.161	0.403	63	79	68	74	21	60 duplicate
19128	124 [734; 1-Monoolioleoylglyce 102	[904; Galactose methoxymamine (6TMS)]	59	0.030	-0.137	19.406	0.352	64	78	89	53	46	125 duplicate
12293	124 [734; 1-Monoolioleoylglyce 18	[590; 1-Acetyl-2-thiohydantoin]	59	0.027	-0.091	25.201	0.365	65	77	77	65	74	105 duplicate
14746	124 [734; 1-Monoolioleoylglyce 40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	59	0.024	-0.095	52.809	0.428	66	76	78	64	136	29 duplicate
19518	124 [734; 1-Monoolioleoylglyce 114	Fructose-6-phosphate	48	0.023	-0.086	16.450	0.438	67	75	76	66	35	24 duplicate
16866	124 [734; 1-Monoolioleoylglyce 63	Glutamine	49	0.020	0.285	20.111	0.391	68	74	39	103	50	72 duplicate
19463	124 [734; 1-Monoolioleoylglyce 112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	58	0.019	-0.127	8.688	0.406	69	73	86	56	12	55 duplicate
18158	124 [734; 1-Monoolioleoylglyce 82	Lysine	38	0.010	0.066	28.276	0.494	70	72	64	78	82	3 duplicate
14125	124 [734; 1-Monoolioleoylglyce 34	Aspartic acid	59	0.010	0.087	50.551	0.350	71	71	62	80	132	128 duplicate
12775	124 [734; 1-Monoolioleoylglyce 22	[690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	47	0.008	-0.070	13.670	0.392	72	70	74	68	23	71 duplicate
18716	124 [734; 1-Monoolioleoylglyce 123	[945; Galactofuranose-6-phosphate (7TMS)]	59	-0.001	-0.040	28.589	0.394	73	69	72	70	84	67 duplicate
9801	124 [734; 1-Monoolioleoylglyce	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	59	-0.015	-0.101	30.517	0.400	75	66	79	63	90	62 original
17789	124 [734; 1-Monoolioleoylglyce 76	Fructose	59	-0.015	-0.289	43.611	0.418	76	67	112	30	121	40 duplicate

18543	124 [734; 1-Monooctylethylene glycol 89	[775; Dopamine (4TMS)]	35	-0.015	0.313	15.849	0.371	77	65	36	106	34	97 duplicate
18544	124 [734; 1-Monooctylethylene glycol 41	[639; Proline (2TMS)]	59	-0.017	0.000	31.937	0.357	78	64	69	73	93	117 duplicate
18544	124 [734; 1-Monooctylethylene glycol 115	Glucose-6-phosphate	57	-0.019	-0.281	42.823	0.461	79	63	107	35	118	8 duplicate
13241	124 [734; 1-Monooctylethylene glycol 26	Citramalic acid	59	-0.019	-0.132	34.830	0.349	80	62	87	55	102	129 duplicate
15610	124 [734; 1-Monooctylethylene glycol 49	[877; Pyrophosphoric acid (4TMS)]	59	-0.023	0.042	14.097	0.361	81	60	66	76	24	112 duplicate
13468	124 [734; 1-Monooctylethylene glycol 28	Malic acid	59	-0.023	-0.176	27.250	0.404	82	61	85	47	81	58 duplicate
18966	124 [734; 1-Monooctylethylene glycol 98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	45	-0.024	0.091	9.272	0.316	83	59	60	82	15	140 duplicate
19491	124 [734; 1-Monooctylethylene glycol 113	Galactose-6-phosphate	57	-0.025	-0.288	19.503	0.418	84	58	110	32	47	39 duplicate
19274	124 [734; 1-Monooctylethylene glycol 106	[733; Threitol (4TMS)]	57	-0.030	-0.150	26.579	0.459	85	57	92	50	78	10 duplicate
12893	124 [734; 1-Monooctylethylene glycol 23	Homoserine	59	-0.031	0.122	24.628	0.385	86	56	57	85	70	81 duplicate
11795	124 [734; 1-Monooctylethylene glycol 14	Fumaric acid	59	-0.044	-0.186	16.570	0.362	87	55	98	44	36	108 duplicate
18659	124 [734; 1-Monooctylethylene glycol 120	[945; Uridine (3TMS)]	49	-0.044	-0.147	28.974	0.392	88	54	91	51	85	70 duplicate
15236	124 [734; 1-Monooctylethylene glycol 45	Homocysteine	56	-0.045	-0.083	6.954	0.339	89	53	75	67	8	134 duplicate
12415	124 [734; 1-Monooctylethylene glycol 19	Alanine (BP) (3TMS)	59	-0.049	-0.138	28.746	0.381	90	52	90	52	88	85 duplicate
10616	124 [734; 1-Monooctylethylene glycol 5	Leucine	41	-0.051	-0.103	15.734	0.413	91	51	80	62	32	50 duplicate
17916	124 [734; 1-Monooctylethylene glycol 78	Mannose	57	-0.056	-0.217	20.182	0.414	92	50	100	42	52	48 duplicate
14231	124 [734; 1-Monooctylethylene glycol 35	Pyroglutamic acid	59	-0.057	-0.343	59.343	0.445	93	49	118	24	140	18 duplicate
18879	124 [734; 1-Monooctylethylene glycol 96	myo-Inositol	47	-0.068	-0.108	4.849	0.327	94	48	83	59	4	138 duplicate
11540	124 [734; 1-Monooctylethylene glycol 12	Glycolic acid	58	-0.072	-0.281	14.755	0.368	95	47	108	34	26	102 duplicate
12656	124 [734; 1-Monooctylethylene glycol 21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	59	-0.074	-0.223	35.082	0.379	96	46	102	40	104	89 duplicate
17241	124 [734; 1-Monooctylethylene glycol 68	[570; Hypoxanthine (2TMS)]	19	-0.076	0.185	4.810	0.389	97	45	50	92	3	75 duplicate
17591	124 [734; 1-Monooctylethylene glycol 73	Glucose methoxyamine (5TMS)]	53	-0.078	-0.221	19.606	0.407	98	44	101	41	48	54 duplicate
17978	124 [734; 1-Monooctylethylene glycol 79	Glucose	59	-0.087	-0.271	52.679	0.394	99	43	106	36	135	66 duplicate
19239	124 [734; 1-Monooctylethylene glycol 105	[705; 2-Ketogluconic acid (5TMS)]	43	-0.092	-0.210	26.774	0.408	100	42	99	43	80	53 duplicate
17384	124 [734; 1-Monooctylethylene glycol 70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	53	-0.094	-0.189	34.976	0.395	101	41	97	45	103	65 duplicate
19816	124 [734; 1-Monooctylethylene glycol 118	[928; Glucopyranose-6-phosphate (6TMS)]	53	-0.097	-0.134	19.771	0.417	102	40	88	54	49	42 duplicate
16383	124 [734; 1-Monooctylethylene glycol 57	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	50	-0.123	-0.160	28.567	0.413	103	39	93	49	83	49 duplicate
17523	124 [734; 1-Monooctylethylene glycol 72	[919; D-Xylopyranose (4TMS)]	58	-0.125	-0.124	20.292	0.393	104	38	85	57	53	69 duplicate
15701	124 [734; 1-Monooctylethylene glycol 50	[746; Ribonic acid-1,4-lactone (3TMS)]	55	-0.134	-0.234	9.235	0.401	105	37	103	39	14	61 duplicate
18741	124 [734; 1-Monooctylethylene glycol 93	[607; Putrescine (4TMS)]	55	-0.137	-0.187	12.887	0.338	106	36	96	48	20	136 duplicate
15043	124 [734; 1-Monooctylethylene glycol 43	[548; Leucine (2TBS)]	55	-0.138	-0.107	23.323	0.378	107	35	82	60	64	90 duplicate
13355	124 [734; 1-Monooctylethylene glycol 27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	48	-0.145	0.123	15.454	0.351	108	34	56	86	31	126 duplicate
18273	124 [734; 1-Monooctylethylene glycol 84	Mannitol	57	-0.152	-0.423	49.729	0.382	109	33	137	5	130	84 duplicate
18693	124 [734; 1-Monooctylethylene glycol 92	[680; Glycerol-2-phosphate (4TMS)]	49	-0.156	-0.337	21.852	0.373	110	32	117	25	57	84 duplicate
14543	124 [734; 1-Monooctylethylene glycol 38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	59	-0.162	-0.304	25.286	0.430	111	31	113	29	75	27 duplicate
9781	124 [734; 1-Monooctylethylene glycol 125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru	59	-0.163	-0.413	49.775	0.373	112	30	135	7	131	93 original
16943	124 [734; 1-Monooctylethylene glycol 64	[789; Tyramine (3TMS)]	58	-0.164	-0.287	20.490	0.357	113	29	109	33	54	116 duplicate
9785	124 [734; 1-Monooctylethylene glycol 129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	54	-0.168	-0.244	24.755	0.410	114	28	104	38	72	52 original
18384	124 [734; 1-Monooctylethylene glycol 86	[793; D-Galactono-1,4-lactone (4TMS)]	56	-0.170	-0.372	37.159	0.439	115	27	125	17	112	23 duplicate
11411	124 [734; 1-Monooctylethylene glycol 11	Succinic acid	59	-0.185	-0.388	25.401	0.379	116	26	131	11	76	86 duplicate
10751	124 [734; 1-Monooctylethylene glycol 6	Glycerol	59	-0.186	-0.349	59.782	0.338	117	25	119	23	141	135 duplicate
13126	124 [734; 1-Monooctylethylene glycol 25	[709; 2,5-Diaminovalerolactam (2TMS)]	43	-0.189	-0.066	17.189	0.403	118	24	73	69	37	59 duplicate
16788	124 [734; 1-Monooctylethylene glycol 82	[812; D-Xylofuranose (4TMS)]	59	-0.196	-0.384	32.572	0.390	119	23	129	13	95	74 duplicate
18491	124 [734; 1-Monooctylethylene glycol 88	Gluconic acid	59	-0.207	-0.358	29.378	0.416	120	22	123	19	86	45 duplicate
18923	124 [734; 1-Monooctylethylene glycol 97	[756; beta-D-Methylglucopyranoside (4TMS)]	47	-0.214	-0.357	36.770	0.388	121	21	122	20	109	78 duplicate
19008	124 [734; 1-Monooctylethylene glycol 99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	39	-0.215	-0.253	15.100	0.473	122	20	105	37	29	6 duplicate
9800	124 [734; 1-Monooctylethylene glycol 134	Isomaltose	59	-0.218	-0.350	43.125	0.417	123	19	120	22	120	41 original
11688	124 [734; 1-Monooctylethylene glycol 13	Uracil	59	-0.219	-0.334	34.565	0.442	124	18	116	26	101	20 duplicate
16055	124 [734; 1-Monooctylethylene glycol 54	[NA]	50	-0.224	-0.382	17.502	0.411	125	17	128	14	39	51 duplicate

17019	124 [734; 1-Monoolioxyglyce	65 [646; 3-Deoxyglucitol (5TMS)]	58 -0.228	-0.330	24.265	0.443	126	16	114	28	66	19 duplicate
13580	124 [734; 1-Monoolioxyglyce	29 Erythritol	59 -0.229	-0.380	21.441	0.437	127	15	127	15	56	26 duplicate
14645	124 [734; 1-Monoolioxyglyce	39 [828; 1-Phenylethanol (1TMS)]	58 -0.232	-0.289	33.435	0.422	128	14	111	31	99	35 duplicate
11921	124 [734; 1-Monoolioxyglyce	15 Alanine	59 -0.234	-0.355	38.053	0.361	129	13	121	21	105	111 duplicate
15331	124 [734; 1-Monoolioxyglyce	46 Arabinose	59 -0.241	-0.393	34.017	0.438	130	12	133	9	100	25 duplicate
16299	124 [734; 1-Monoolioxyglyce	58 [829; Orolic acid (3TMS)]	59 -0.251	-0.401	22.229	0.424	131	11	134	8	59	33 duplicate
13010	124 [734; 1-Monoolioxyglyce	24 [725; 2-Ketotectonic acid (2TMS)]	59 -0.258	-0.379	50.644	0.426	132	10	126	16	133	31 duplicate
19168	124 [734; 1-Monoolioxyglyce	103 [646; Ethylamine (2TMS)]	58 -0.266	-0.414	29.673	0.355	133	9	138	6	87	121 duplicate
18438	124 [734; 1-Monoolioxyglyce	87 [845; beta-D-Glucopyranose (5TMS)]	57 -0.266	-0.359	52.968	0.388	134	8	124	18	137	77 duplicate
12046	124 [734; 1-Monoolioxyglyce	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	59 -0.266	-0.390	36.433	0.447	135	7	132	10	108	16 duplicate
18039	124 [734; 1-Monoolioxyglyce	80 [772; D-Glucose (5TMS)]	57 -0.269	-0.332	48.472	0.332	136	6	115	27	129	137 duplicate
12170	124 [734; 1-Monoolioxyglyce	17 [700; 2-methyl-1,2-propanediol (2TMS)]	59 -0.295	-0.460	36.209	0.387	137	5	138	4	106	80 duplicate
18844	124 [734; 1-Monoolioxyglyce	91 [766; beta-D-Methylglucopyranoside (4TMS)]	59 -0.305	-0.498	30.766	0.369	138	4	139	3	91	99 duplicate
15425	124 [734; 1-Monoolioxyglyce	47 [NA]	59 -0.320	-0.386	25.137	0.419	139	3	130	12	73	37 duplicate
19089	124 [734; 1-Monoolioxyglyce	101 [832; Dopamine (4TMS)]	-59 -0.362	-0.511	26.562	0.369	140	2	140	2	77	100 duplicate
10068	124 [734; 1-Monoolioxyglyce	1 [938; Sulfuric acid (2TMS)]	34 -0.437	-0.536	18.029	0.449	141	1	141	1	41	13 duplicate
16789	125 [892; Sucrose (8TMS);	62 [812; D-Xylofuranose (4TMS)]	64 0.683	0.868	19.107	0.589	1	141	10	132	34	22 duplicate
14835	125 [892; Sucrose (8TMS);	86 [793; D-Galactono-1,4-lactone (4TMS)]	61 0.854	0.921	19.106	0.616	2	140	3	139	33	11 duplicate
14232	125 [892; Sucrose (8TMS);	35 Pyrogulonic acid	64 0.638	0.942	12.907	0.630	3	139	1	141	11	7 duplicate
12657	125 [892; Sucrose (8TMS);	21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	61 0.815	0.680	17.207	0.505	4	138	41	101	27	68 duplicate
17917	125 [892; Sucrose (8TMS);	78 Mannose	62 0.591	0.831	32.463	0.546	5	137	16	126	99	43 duplicate
13011	125 [892; Sucrose (8TMS);	24 [725; 2-Ketobutanoic acid (2TMS)]	64 0.566	0.776	26.353	0.553	7	135	26	116	65	39 duplicate
15332	125 [892; Sucrose (8TMS);	11 Succinic acid	64 0.578	0.881	21.327	0.631	8	134	8	134	40	6 duplicate
14512	125 [892; Sucrose (8TMS);	46 Arabinose	64 0.577	0.776	26.353	0.553	7	135	26	116	65	39 duplicate
17790	125 [892; Sucrose (8TMS);	76 Fructose	64 0.574	0.940	8.093	0.619	9	133	2	140	5	10 duplicate
14207	125 [892; Sucrose (8TMS);	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	64 0.570	0.710	10.935	0.530	10	132	39	103	7	54 duplicate
12047	125 [892; Sucrose (8TMS);	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	64 0.568	0.764	15.659	0.589	11	131	28	113	20	23 duplicate
13469	125 [892; Sucrose (8TMS);	28 Malic acid	64 0.566	0.720	24.552	0.537	12	130	36	108	57	48 duplicate
17592	125 [892; Sucrose (8TMS);	73 [708; Glucose methoxyamine (5TMS)]	57 0.565	0.781	29.978	0.506	13	129	25	117	81	66 duplicate
11798	125 [892; Sucrose (8TMS);	14 Fumaric acid	64 0.563	0.722	35.554	0.547	14	128	35	107	109	41 duplicate
14544	125 [892; Sucrose (8TMS);	65 [646; 3-Deoxyglucitol (5TMS)]	63 0.559	0.843	32.251	0.636	15	127	14	128	97	48 duplicate
17020	125 [892; Sucrose (8TMS);	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	64 0.558	0.738	28.659	0.542	16	126	32	110	67	48 duplicate
19680	125 [892; Sucrose (8TMS);	120 [945; Uridine (3TMS)]	54 0.550	0.364	21.483	0.521	17	125	68	74	41	61 duplicate
18482	125 [892; Sucrose (8TMS);	88 Gluconic acid	64 0.550	0.767	23.561	0.577	18	124	27	115	53	27 duplicate
14646	125 [892; Sucrose (8TMS);	39 [829; 1-Phenylethanol (1TMS)]	63 0.545	0.736	21.174	0.563	19	123	33	109	39	34 duplicate
19545	125 [892; Sucrose (8TMS);	115 Glucose-6-phosphate	62 0.543	0.911	8.265	0.607	20	122	4	138	6	13 duplicate
16300	125 [892; Sucrose (8TMS);	56 [829; Orolic acid (3TMS)]	64 0.542	0.863	32.349	0.642	21	121	12	130	98	1 duplicate
32581	125 [892; Sucrose (8TMS);	29 Erythritol	64 0.540	0.711	30.499	0.529	22	120	38	104	85	56 duplicate
12171	125 [892; Sucrose (8TMS);	17 [700; 2-methyl-1,2-propanediol (2TMS)]	64 0.534	0.783	16.082	0.547	23	119	24	118	21	42 duplicate
19275	125 [892; Sucrose (8TMS);	106 [733; Threitol (4TMS)]	62 0.527	0.807	25.526	0.599	24	118	19	123	61	18 duplicate
9816	125 [892; Sucrose (8TMS);	134 Isomaltose	64 0.521	0.840	11.923	0.634	25	117	15	127	9	5 original
10752	125 [892; Sucrose (8TMS);	6 Glycerol	64 0.512	0.895	13.908	0.554	26	116	6	138	13	38 duplicate
17385	125 [892; Sucrose (8TMS);	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57 0.511	0.732	13.196	0.532	27	115	34	108	12	53 duplicate
12276	125 [892; Sucrose (8TMS);	22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52 0.508	0.610	36.551	0.471	28	114	48	94	111	79 duplicate
15702	125 [892; Sucrose (8TMS);	50 [746; Ribonic acid-1,4-lactone (3TMS)]	61 0.508	0.713	45.400	0.506	29	113	37	105	137	67 duplicate
16056	125 [892; Sucrose (8TMS);	54 [NA]	55 0.507	0.785	36.470	0.562	30	112	23	119	110	35 duplicate
11669	125 [892; Sucrose (8TMS);	13 Urcal	64 0.507	0.766	17.979	0.589	31	111	28	114	30	24 duplicate
3242	125 [892; Sucrose (8TMS);	26 Citramalic acid	64 0.499	0.638	17.809	0.461	32	110	43	89	29	81 duplicate
		129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-Glc]										
9811	125 [892; Sucrose (8TMS);	113 Galactose-6-phosphate	59 0.492	0.789	29.752	0.604	33	109	22	120	80	16 original
18492	125 [892; Sucrose (8TMS);		62 0.483	0.904	32.239	0.573	34	108	5	137	95	30 duplicate

12294	125 [892; Sucrose (8TMS); $\epsilon$ 18 [590; 1-Acetyl-2-thiohydantoin]	64	0.482	0.562	26.802	0.420	35	107	55	87	69	101 duplicate
9814	125 [892; Sucrose (8TMS); $\epsilon$ 132 [895; Isomaltose methoxyamine (8TMS)]	42	0.466	0.635	37.008	0.541	36	106	44	98	112	47 original
11541	125 [892; Sucrose (8TMS); $\epsilon$ 12 Glycic acid	63	0.463	0.588	37.780	0.485	37	105	52	90	113	75 duplicate
18519	125 [892; Sucrose (8TMS); $\epsilon$ 114 Fructose-6-phosphate	53	0.463	0.865	31.328	0.603	38	104	11	131	91	17 duplicate
19129	125 [892; Sucrose (8TMS); $\epsilon$ 102 [904; Galactose methoxyamine (5TMS)]	64	0.454	0.474	32.729	0.464	40	102	62	80	101	80 duplicate
16394	125 [892; Sucrose (8TMS); $\epsilon$ 57 [757; 2-Desoxy-pentose-3-ylose dimethoxyamine (2TMS)]	55	0.452	0.829	26.203	0.604	41	101	17	125	64	14 duplicate
12416	125 [892; Sucrose (8TMS); $\epsilon$ 19 Alanine (BP) (3TMS)	64	0.450	0.803	21.874	0.524	42	100	21	121	44	58 duplicate
18464	125 [892; Sucrose (8TMS); $\epsilon$ 112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	83	0.428	0.494	43.805	0.448	43	99	59	83	135	87 duplicate
19680	125 [892; Sucrose (8TMS); $\epsilon$ 121 [657; Erythritol (4TMS)]	55	0.421	0.631	39.368	0.552	44	98	46	96	122	40 duplicate
19050	125 [892; Sucrose (8TMS); $\epsilon$ 100 [857; Mannitol (6TMS)]	64	0.415	0.481	25.522	0.452	45	97	60	82	60	86 duplicate
19204	125 [892; Sucrose (8TMS); $\epsilon$ 104 [795; Erythritol (4TMS)]	63	0.402	0.647	28.927	0.507	46	96	42	100	76	85 duplicate
18594	125 [892; Sucrose (8TMS); $\epsilon$ 117 [724; Glycerol (3TMS)]	58	0.396	0.580	31.102	0.504	47	95	50	92	89	69 duplicate
17659	125 [892; Sucrose (8TMS); $\epsilon$ 74 [812; Tetradecanoic acid (1TMS)]	64	0.384	0.455	32.249	0.412	48	94	64	78	96	104 duplicate
19717	125 [892; Sucrose (8TMS); $\epsilon$ 123 [945; Galactofuranose-6-phosphate (7TMS)]	64	0.377	0.751	22.848	0.522	49	93	31	111	49	60 duplicate
18439	125 [892; Sucrose (8TMS); $\epsilon$ 87 [945; beta-D-Glucopyranose (5TMS)]	62	0.375	0.859	7.491	0.522	50	92	13	129	4	59 duplicate
19405	125 [892; Sucrose (8TMS); $\epsilon$ 110 [715; Erythritol (4TMS)]	54	0.368	0.701	34.343	0.576	51	91	40	102	108	28 duplicate
19689	125 [892; Sucrose (8TMS); $\epsilon$ 122 [644; Erythritol (4TMS)]	52	0.365	0.576	40.678	0.518	52	90	53	89	125	63 duplicate
14847	125 [892; Sucrose (8TMS); $\epsilon$ 41 [639; Proline (2TMS)]	64	0.344	0.620	20.223	0.479	53	89	47	95	36	77 duplicate
9817	125 [892; Sucrose (8TMS); $\epsilon$ 135 [902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	0.338	0.316	22.003	0.409	54	88	69	73	45	105 original
17879	125 [892; Sucrose (8TMS); $\epsilon$ 79 Glucose	64	0.327	0.878	6.917	0.572	55	87	9	133	1	31 duplicate
16944	125 [892; Sucrose (8TMS); $\epsilon$ 84 [789; Tyramine (3TMS)]	63	0.324	0.601	31.153	0.398	56	86	49	93	90	109 duplicate
11922	125 [892; Sucrose (8TMS); $\epsilon$ 15 Alanine	64	0.311	0.755	15.388	0.594	57	85	30	112	18	20 duplicate
15141	125 [892; Sucrose (8TMS); $\epsilon$ 44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	0.308	0.552	28.332	0.535	58	84	57	85	75	51 duplicate
19167	125 [892; Sucrose (8TMS); $\epsilon$ 103 [648; Ethylamine (2TMS)]	63	0.302	0.574	26.725	0.502	59	83	54	88	68	70 duplicate
18330	125 [892; Sucrose (8TMS); $\epsilon$ 85 [528; Methylcitric acid (4TMS)]	48	0.301	0.407	24.886	0.344	60	82	67	75	58	135 duplicate
19009	125 [892; Sucrose (8TMS); $\epsilon$ 99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	0.298	0.635	32.022	0.564	61	81	45	97	94	33 duplicate
19570	125 [892; Sucrose (8TMS); $\epsilon$ 116 [882; Pseudouridine (5TMS)]	30	0.297	0.037	24.079	0.366	62	80	79	63	54	129 duplicate
18880	125 [892; Sucrose (8TMS); $\epsilon$ 96 myo-Inositol	49	0.293	0.226	41.745	0.330	63	79	72	70	129	139 duplicate
18217	125 [892; Sucrose (8TMS); $\epsilon$ 83 Sorbitol	58	0.288	-0.128	17.202	0.341	64	78	86	56	26	136 duplicate
18040	125 [892; Sucrose (8TMS); $\epsilon$ 80 [772; D-Glucose (5TMS)]	62	0.258	0.809	7.325	0.509	65	77	18	124	3	64 duplicate
19090	125 [892; Sucrose (8TMS); $\epsilon$ 101 [832; Dopamine (4TMS)]	64	0.241	0.517	28.119	0.489	66	76	58	84	74	74 duplicate
18645	125 [892; Sucrose (8TMS); $\epsilon$ 91 [766; beta-D-Methylglucopyranoside (4TMS)]	64	0.227	0.477	28.142	0.459	67	75	61	81	77	82 duplicate
18694	125 [892; Sucrose (8TMS); $\epsilon$ 92 [680; Glycerol-2-phosphate (4TMS)]	54	0.224	0.884	30.111	0.545	68	74	7	135	83	45 duplicate
9815	125 [892; Sucrose (8TMS); $\epsilon$ 133 [855; Squalene]	64	0.208	0.110	29.709	0.357	69	73	77	65	79	132 original
9808	125 [892; Sucrose (8TMS); $\epsilon$ 126 [559; Erythritol (4TMS)]	45	0.202	0.194	32.625	0.577	70	72	73	69	100	28 original
10067	125 [892; Sucrose (8TMS); $\epsilon$ 1 [938; Sulfuric acid (2TMS)]	38	0.190	0.460	27.907	0.575	71	71	63	79	72	29 duplicate
9810	125 [892; Sucrose (8TMS); $\epsilon$ 128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.143	0.447	26.045	0.536	72	70	65	77	63	49 original
19435	125 [892; Sucrose (8TMS); $\epsilon$ 111 [583; Erythritol (4TMS)]	42	0.134	0.243	43.857	0.435	73	69	71	71	136	93 duplicate
19374	125 [892; Sucrose (8TMS); $\epsilon$ 109 Octadecanoic acid	64	0.097	0.258	18.887	0.428	74	68	70	72	32	97 duplicate
9820	125 [892; Sucrose (8TMS); $\epsilon$ 138 [674; Ergosterol (1TMS)]	46	0.088	0.087	38.273	0.429	75	67	78	64	117	98 original
18924	125 [892; Sucrose (8TMS); $\epsilon$ 97 [756; beta-D-Methylglucopyranoside (4TMS)]	52	0.083	0.559	20.509	0.546	76	66	58	86	37	44 duplicate
9822	125 [892; Sucrose (8TMS); $\epsilon$ 140 [892; Ergosta-7,22-dien-3-ol (1TMS)]	49	0.075	-0.027	38.447	0.379	77	65	81	61	121	119 original
19617	125 [892; Sucrose (8TMS); $\epsilon$ 118 [928; Glucopyranose-6-phosphate (8TMS)]	58	0.051	0.446	33.005	0.440	78	64	68	76	102	90 duplicate
15426	125 [892; Sucrose (8TMS); $\epsilon$ 47 [NA]	64	0.044	0.161	30.926	0.372	79	63	74	68	87	123 duplicate
18274	125 [892; Sucrose (8TMS); $\epsilon$ 84 Mannitol	62	0.043	0.148	15.104	0.401	80	62	75	67	17	107 duplicate
18789	125 [892; Sucrose (8TMS); $\epsilon$ 94 Hexadecanoic acid	64	0.025	0.128	16.814	0.418	81	61	76	68	24	102 duplicate
19240	125 [892; Sucrose (8TMS); $\epsilon$ 105 [705; 2-Ketogluconic acid (5TMS)]	48	0.000	0.011	27.862	0.528	82	60	80	62	71	57 duplicate
9821	125 [892; Sucrose (8TMS); $\epsilon$ 139 [700; Ergosta-5,7-dien-3-ol]	38	-0.016	-0.222	38.187	0.349	83	59	91	51	115	133 original
9823	125 [892; Sucrose (8TMS); $\epsilon$ 141 Lanosta-8,24-dien-3-beta-ol	61	-0.016	-0.239	40.440	0.370	84	58	92	50	123	126 original

17455	125 [892; Sucrose (8TMS); ε 71	[731; Erythrose (3TMS)]	64	-0.031	-0.197	22.701	0.369	85	57	89	53	46	127 duplicate
9809	125 [892; Sucrose (8TMS); ε 127	[777; Fructose-6-phosphate methoxyamine (8TMS)]	39	-0.034	-0.083	27.701	0.567	86	56	83	59	70	32 original
15969	125 [892; Sucrose (8TMS); ε 53	Glycerol-2-phosphate	51	-0.044	-0.199	38.413	0.368	87	55	90	52	120	128 duplicate
10481	125 [892; Sucrose (8TMS); ε 4	Phosphoric acid	51	-0.048	-0.157	13.910	0.274	88	54	88	54	14	141 duplicate
9819	125 [892; Sucrose (8TMS); ε 137	Ergosterol	64	-0.051	-0.260	25.505	0.371	89	53	94	48	59	125 original
9812	125 [892; Sucrose (8TMS); ε 130	Trehalose	63	-0.073	-0.114	11.821	0.338	90	52	84	58	8	138 original
17524	125 [892; Sucrose (8TMS); ε 72	[919; D-Xylopyranose (4TMS)]	63	-0.077	-0.082	34.116	0.345	91	51	82	60	108	134 duplicate
	125 [892; Sucrose (8TMS); ε 58	[636; 4R-Acetamido-2,3-Z-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	-0.092	-0.120	21.859	0.339	92	50	85	57	43	137 duplicate
18595	125 [892; Sucrose (8TMS); ε 90	[910; 9-Z)-Hexadecenoic acid (1TMS)]	64	-0.111	-0.382	29.357	0.382	93	48	102	40	78	117 duplicate
14337	125 [892; Sucrose (8TMS); ε 36	[596; N-Acetylglutamic acid (2TMS)]	64	-0.118	-0.289	15.036	0.362	94	48	96	46	16	131 duplicate
19639	125 [892; Sucrose (8TMS); ε 119	[931; myo-Inositol-2-phosphate (7TMS)]	64	-0.155	-0.527	30.390	0.445	95	47	112	30	84	88 duplicate
17725	125 [892; Sucrose (8TMS); ε 75	Lysine	64	-0.157	-0.242	16.668	0.378	96	46	93	49	23	120 duplicate
	125 [892; Sucrose (8TMS); ε 124	[734; 1-Monoleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]	59	-0.163	-0.413	49.775	0.373	97	45	103	39	140	121 duplicate
17095	125 [892; Sucrose (8TMS); ε 66	Glyceric acid-3-phosphate	64	-0.171	-0.311	33.450	0.372	98	44	97	45	104	122 duplicate
19309	125 [892; Sucrose (8TMS); ε 107	9-Z)-Octadecenoic acid	64	-0.177	-0.532	21.559	0.380	99	43	113	29	42	118 duplicate
18987	125 [892; Sucrose (8TMS); ε 98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	48	-0.188	-0.468	41.789	0.386	100	42	106	36	130	115 duplicate
19342	125 [892; Sucrose (8TMS); ε 108	Octadecenoic acid	64	-0.189	-0.480	34.310	0.393	101	41	107	35	107	111 duplicate
10886	125 [892; Sucrose (8TMS); ε 7	Threonine	64	-0.195	-0.331	12.868	0.372	102	40	98	44	10	124 duplicate
18742	125 [892; Sucrose (8TMS); ε 93	[607; Putrescine (4TMS)]	60	-0.195	-0.134	43.058	0.385	103	39	87	55	134	116 duplicate
13356	125 [892; Sucrose (8TMS); ε 27	[815; (E)-4-Methyl-5-hydroxy-3-pentan-2-one (1TMS)]	53	-0.215	-0.487	41.023	0.420	104	38	108	34	127	100 duplicate
10208	125 [892; Sucrose (8TMS); ε 2	Serine	62	-0.234	-0.352	26.374	0.391	105	37	100	42	68	113 duplicate
9818	125 [892; Sucrose (8TMS); ε 136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.265	-0.362	17.710	0.431	106	36	101	41	28	95 original
16710	125 [892; Sucrose (8TMS); ε 61	NA	64	-0.288	-0.601	31.075	0.499	107	35	123	19	88	72 duplicate
17169	125 [892; Sucrose (8TMS); ε 67	Citric acid	64	-0.290	-0.609	14.391	0.438	108	34	124	18	15	91 duplicate
16630	125 [892; Sucrose (8TMS); ε 60	Glycerol-3-phosphate	64	-0.312	-0.566	16.988	0.472	109	33	119	23	25	78 duplicate
12894	125 [892; Sucrose (8TMS); ε 23	Homoserine	64	-0.316	-0.574	31.846	0.500	110	32	122	20	92	71 duplicate
15044	125 [892; Sucrose (8TMS); ε 43	[548; Leucine (2TMS)]	60	-0.321	-0.278	28.024	0.454	111	31	95	47	73	85 duplicate
16667	125 [892; Sucrose (8TMS); ε 63	Glutamine	52	-0.333	-0.894	37.922	0.640	112	30	136	6	114	2 duplicate
11019	125 [892; Sucrose (8TMS); ε 8	Isoleucine	55	-0.335	-0.342	23.269	0.313	113	29	99	43	50	140 duplicate
14441	125 [892; Sucrose (8TMS); ε 37	Phenylalanine	64	-0.346	-0.588	15.398	0.424	114	28	120	22	19	98 duplicate
13802	125 [892; Sucrose (8TMS); ε 31	[622; Parabenic acid (2TMS)]	64	-0.353	-0.493	38.272	0.434	115	27	109	33	116	94 duplicate
15881	125 [892; Sucrose (8TMS); ε 52	NA	46	-0.355	-0.872	41.586	0.596	116	26	135	7	128	18 duplicate
11151	125 [892; Sucrose (8TMS); ε 9	Proline	63	-0.368	-0.436	24.301	0.392	117	25	104	38	55	112 duplicate
13127	125 [892; Sucrose (8TMS); ε 25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.376	-0.543	38.323	0.529	118	24	115	27	119	55 duplicate
17242	125 [892; Sucrose (8TMS); ε 68	[570; Hypoxanthine (2TMS)]	20	-0.411	-0.922	25.897	0.535	119	23	138	4	62	50 duplicate
13911	125 [892; Sucrose (8TMS); ε 32	[729; N,N-Dimethyllysine methyl ester]	63	-0.414	-0.551	41.009	0.490	120	22	116	26	126	73 duplicate
9813	125 [892; Sucrose (8TMS); ε 131	[626; 5-Methylthioadenosine (3TMS)]	55	-0.415	-0.695	42.323	0.561	121	21	129	13	131	37 original
14126	125 [892; Sucrose (8TMS); ε 34	Aspartic acid	64	-0.438	-0.468	16.582	0.446	122	20	105	37	22	88 duplicate
15611	125 [892; Sucrose (8TMS); ε 49	[877; Pyrophosphoric acid (4TMS)]	64	-0.463	-0.642	47.732	0.437	123	19	126	16	138	92 duplicate
10344	125 [892; Sucrose (8TMS); ε 3	Ethanolamine	62	-0.467	-0.816	38.303	0.593	124	18	131	11	118	21 duplicate
14019	125 [892; Sucrose (8TMS); ε 33	Methionine	64	-0.468	-0.527	31.939	0.455	125	17	111	31	93	83 duplicate
15792	125 [892; Sucrose (8TMS); ε 51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.469	-0.619	40.485	0.396	126	16	125	17	124	110 duplicate
18100	125 [892; Sucrose (8TMS); ε 81	Tyrosine	64	-0.483	-0.766	21.135	0.604	127	15	130	12	38	15 duplicate
13692	125 [892; Sucrose (8TMS); ε 30	[815; Ethyl-3(2H)-thiophenone]	64	-0.486	-0.512	19.544	0.399	128	14	110	32	35	108 duplicate
15237	125 [892; Sucrose (8TMS); ε 45	Homocysteine	61	-0.491	-0.541	48.638	0.364	129	13	114	28	139	130 duplicate
16142	125 [892; Sucrose (8TMS); ε 55	[612; 4-Aminobutyric acid (2TBS)]	43	-0.499	-0.956	42.830	0.534	130	12	140	2	133	52 duplicate
17314	125 [892; Sucrose (8TMS); ε 69	Arginine	60	-0.501	-0.689	23.394	0.519	131	11	128	14	52	62 duplicate
16549	125 [892; Sucrose (8TMS); ε 59	Ornithine; Arginine	64	-0.514	-0.554	18.730	0.416	132	10	117	25	31	103 duplicate
15519	125 [892; Sucrose (8TMS); ε 48	Asparagine	64	-0.530	-0.859	34.057	0.608	133	9	134	8	105	12 duplicate

11282	125 [892; Sucrose (8TMS); ε 10	Glycine	64	-0.540	-0.826	22,745	0.639	134	8	133	9	47	3 duplicate
14946	125 [892; Sucrose (8TMS); ε 42	Glutamic acid	60	-0.542	-0.573	24,531	0.404	135	7	121	21	56	106 duplicate
10617	125 [892; Sucrose (8TMS); ε 5	Leucine	45	-0.543	-0.565	29,990	0.388	136	6	118	24	82	114 duplicate
18544	125 [892; Sucrose (8TMS); ε 89	[776; Dopamine (4TMS)]	35	-0.563	-0.872	33,127	0.561	137	5	141	1	103	38 duplicate
	125 [892; Sucrose (8TMS); ε 77	[826; beta-[[[5-methyl-2-thienyl]methyl]amino]-benzeneacetic acid methyl ester]	62	-0.564	-0.687	22,757	0.454	138	4	127	15	48	84 duplicate
18159	125 [892; Sucrose (8TMS); ε 82	Lysine	39	-0.611	-0.912	23,318	0.620	139	3	137	5	51	9 duplicate
18835	125 [892; Sucrose (8TMS); ε 95	[770; 3,4,6-Trisubstituted phenylalanine (5TMS)]	50	-0.623	-0.821	42,822	0.485	140	2	132	10	132	76 duplicate
	125 [892; Sucrose (8TMS); ε 20	[619; 2-(3',4'-Bisubstituted phenyl)-2-oxoethylamine (4TMS)]	31	-0.738	-0.954	30,773	0.583	141	1	139	3	86	25 duplicate
19700	126 [559; Erythritol (4TMS)]	122 [644; Erythritol (4TMS)]	45	0.810	0.930	5,943	0.677	1	140	4	137	11	6 duplicate
19595	126 [559; Erythritol (4TMS)]	117 [724; Glyceral (3TMS)]	44	0.793	0.953	3,884	0.661	2	138	1	140	3	10 duplicate
19681	126 [559; Erythritol (4TMS)]	121 [657; Erythritol (4TMS)]	44	0.793	0.933	5,500	0.629	3	139	3	138	6	28 duplicate
19406	126 [559; Erythritol (4TMS)]	110 [715; Erythritol (4TMS)]	44	0.792	0.948	3,192	0.729	4	137	2	139	1	1 duplicate
19276	126 [559; Erythritol (4TMS)]	108 [733; Threitol (4TMS)]	44	0.770	0.902	9,688	0.710	5	136	7	134	42	2 duplicate
15142	126 [559; Erythritol (4TMS)]	44 [910; 2-Ketoglucuronic acid methoxymethylamine (4TMS)]	45	0.758	0.920	7,137	0.637	6	135	5	136	20	25 duplicate
17791	126 [559; Erythritol (4TMS)]	76 Fructose	45	0.723	0.888	26,294	0.605	7	134	8	133	125	36 duplicate
14748	126 [559; Erythritol (4TMS)]	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	45	0.873	0.822	31,194	0.588	8	133	13	128	132	46 duplicate
18051	126 [559; Erythritol (4TMS)]	100 [857; Mannitol (6TMS)]	45	0.848	0.769	9,446	0.597	9	132	17	124	40	40 duplicate
18546	126 [559; Erythritol (4TMS)]	115 Glucose-6-phosphate	45	0.844	0.833	25,049	0.653	10	131	12	129	121	18 duplicate
142233	126 [559; Erythritol (4TMS)]	35 Pyroglutamic acid	45	0.828	0.791	38,515	0.614	11	130	15	126	139	32 duplicate
1919130	126 [559; Erythritol (4TMS)]	102 [904; Galactose methoxymethylamine (5TMS)]	45	0.824	0.730	5,960	0.580	12	129	19	122	13	54 duplicate
17680	126 [559; Erythritol (4TMS)]	74 [912; Tetradecanoic acid (1TMS)]	45	0.616	0.857	5,483	0.517	13	128	11	130	5	83 duplicate
18790	126 [559; Erythritol (4TMS)]	94 Hexadecanoic acid	45	0.572	0.864	18,669	0.598	14	127	10	131	105	38 duplicate
13470	126 [559; Erythritol (4TMS)]	28 Malic acid	45	0.556	0.764	10,240	0.546	15	126	18	123	45	74 duplicate
19375	126 [559; Erythritol (4TMS)]	109 Octadecanoic acid	45	0.545	0.876	19,641	0.603	16	125	9	132	110	37 duplicate
9838	126 [559; Erythritol (4TMS)]	141 Lanosta-8,24-dien-3-beta-ol	42	0.538	0.777	8,394	0.537	17	124	16	125	31	79 original
	126 [559; Erythritol (4TMS)]	135											
9832	126 [559; Erythritol (4TMS)]	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	45	0.533	0.695	12,353	0.516	18	123	23	118	60	85 original
17918	126 [559; Erythritol (4TMS)]	78 Mannose	43	0.506	0.699	6,036	0.588	19	122	22	119	15	48 duplicate
9837	126 [559; Erythritol (4TMS)]	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	32	0.504	0.719	11,338	0.426	20	121	21	120	53	118 original
19640	126 [559; Erythritol (4TMS)]	119 [931; myo-inositol-2-phosphate (7TMS)]	45	0.489	0.644	6,167	0.511	21	120	31	110	16	88 duplicate
19465	126 [559; Erythritol (4TMS)]	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (8TMS)]	45	0.483	0.640	11,138	0.478	22	119	33	108	51	96 duplicate
11797	126 [559; Erythritol (4TMS)]	14 Fumaric acid	45	0.463	0.682	5,906	0.570	23	118	28	115	9	61 duplicate
9834	126 [559; Erythritol (4TMS)]	137 Ergosterol	45	0.461	0.494	11,685	0.469	24	117	59	82	56	99 original
18331	126 [559; Erythritol (4TMS)]	85 [529; Methylcitric acid (4TMS)]	29	0.458	0.815	5,951	0.589	25	116	14	127	12	45 duplicate
17593	126 [559; Erythritol (4TMS)]	73 [708; Glucose methoxymethylamine (5TMS)]	38	0.457	0.719	6,021	0.543	26	115	20	121	14	76 duplicate
9829	126 [559; Erythritol (4TMS)]	132 [895; Isomaltose methoxymethylamine (8TMS)]	38	0.440	0.654	8,822	0.548	27	114	30	111	34	73 original
3243	126 [559; Erythritol (4TMS)]	26 Citramalic acid	45	0.428	0.627	15,988	0.515	28	113	34	107	87	86 duplicate
9835	126 [559; Erythritol (4TMS)]	138 [674; Ergosterol (1TMS)]	32	0.419	0.687	11,949	0.441	29	112	24	117	59	111 original
12777	126 [559; Erythritol (4TMS)]	22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	40	0.408	0.680	5,828	0.615	30	111	27	114	7	31 duplicate
14545	126 [559; Erythritol (4TMS)]	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	45	0.406	0.677	9,004	0.661	31	110	28	113	36	12 duplicate
12295	126 [559; Erythritol (4TMS)]	18 [590; 1-Acetyl-2-thiohydantoin]	45	0.402	0.555	8,729	0.511	32	109	43	98	33	89 duplicate
9824	126 [559; Erythritol (4TMS)]	127 [777; Fructose-6-phosphate methoxymethylamine (6TMS)]	39	0.401	0.515	5,849	0.452	33	108	57	84	8	107 original
12658	126 [559; Erythritol (4TMS)]	21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	45	0.398	0.490	16,632	0.560	34	107	60	81	92	65 duplicate
18398	126 [559; Erythritol (4TMS)]	86 [793; D-Galactono-1,4-lactone (4TMS)]	42	0.368	0.685	21,476	0.698	35	106	25	116	115	3 duplicate
	126 [559; Erythritol (4TMS)]	[734; 1-Monoolioxyglycerol (2TMS); 1-Monoheptadecanoylglycerol (1TMS)]	40	0.367	0.520	17,836	0.496	36	105	55	86	99	93 duplicate
19735	126 [559; Erythritol (4TMS)]	113 Glucose-6-phosphate	45	0.354	0.671	6,365	0.657	37	104	28	112	17	13 duplicate
9893	126 [559; Erythritol (4TMS)]	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	43	0.353	0.526	8,985	0.496	38	103	50	91	35	92 original
18861	126 [559; Erythritol (4TMS)]	120 [945; Uridine (3TMS)]	44	0.347	0.070	13,769	0.577	39	102	84	57	75	58 duplicate

16790	126 [559; Erythritol (4TMS)]	62 [812; D-Xylofuranose (4TMS)]	45 0.343	0.535	15,004	0.670	40	101	48	93	79	7 duplicate
19436	126 [559; Erythritol (4TMS)]	111 [593; Erythritol (4TMS)]	36 0.330	0.449	18,378	0.346	41	100	62	79	89	135 duplicate
18218	126 [559; Erythritol (4TMS)]	83 Sorbitol	39 0.323	0.239	18,399	0.424	42	99	75	68	101	117 duplicate
19205	126 [559; Erythritol (4TMS)]	104 [795; Erythritol (4TMS)]	44 0.319	0.564	7,662	0.551	43	98	40	101	22	72 duplicate
17456	126 [559; Erythritol (4TMS)]	71 [731; Erythrose (3TMS)]	45 0.319	0.540	11,788	0.538	44	97	47	94	57	78 duplicate
11542	126 [559; Erythritol (4TMS)]	12 Glycemic acid	45 0.313	0.588	6,669	0.588	45	96	37	104	18	47 duplicate
13582	126 [559; Erythritol (4TMS)]	29 Erythritol	45 0.305	0.525	7,081	0.639	46	94	51	90	19	23 duplicate
11413	126 [559; Erythritol (4TMS)]	11 Succinic acid	45 0.305	0.523	9,408	0.569	47	95	53	88	39	82 duplicate
17386	126 [559; Erythritol (4TMS)]	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	38 0.300	0.231	18,775	0.528	48	93	77	64	107	81 duplicate
19520	126 [559; Erythritol (4TMS)]	114 Fructose-6-phosphate	40 0.297	0.615	5,265	0.648	49	92	35	108	4	20 duplicate
19310	126 [559; Erythritol (4TMS)]	107 9-(Z)-Octadecenoic acid	45 0.295	0.357	13,073	0.403	50	91	67	74	68	124 duplicate
14848	126 [559; Erythritol (4TMS)]	41 [639; Proline (2TMS)]	45 0.289	0.530	13,924	0.556	51	90	49	92	76	69 duplicate
15703	126 [559; Erythritol (4TMS)]	50 [746; Ribonic acid-1,4-lactone (3TMS)]	45 0.285	0.517	11,187	0.593	52	89	56	85	52	43 duplicate
14647	126 [559; Erythritol (4TMS)]	39 [829; 1-Phenylethanol (1TMS)]	45 0.277	0.642	16,867	0.612	53	88	32	109	93	35 duplicate
12417	126 [559; Erythritol (4TMS)]	19 Alanine (BP) (3TMS)	45 0.273	0.580	12,835	0.557	54	87	39	102	62	68 duplicate
9830	126 [559; Erythritol (4TMS)]	133 [855; Squalene]	45 0.269	0.391	8,212	0.404	55	86	65	76	29	123 original
9826	126 [559; Erythritol (4TMS)]	129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	45 0.263	0.548	9,914	0.648	56	85	45	96	44	21 original
13012	126 [559; Erythritol (4TMS)]	24 [725; 2-Ketododecanoic acid (2TMS)]	45 0.261	0.559	31,324	0.679	57	84	41	100	133	5 duplicate
16301	126 [559; Erythritol (4TMS)]	56 [829; Orotic acid (3TMS)]	45 0.257	0.546	7,818	0.655	58	83	46	95	23	16 duplicate
18695	126 [559; Erythritol (4TMS)]	92 [680; Glycerol-2-phosphate (4TMS)]	45 0.238	0.260	8,551	0.553	59	82	73	68	32	70 duplicate
18596	126 [559; Erythritol (4TMS)]	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	45 0.236	0.284	7,845	0.385	60	81	72	69	24	130 duplicate
9833	126 [559; Erythritol (4TMS)]	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17 0.221	0.523	3,476	0.386	61	80	54	87	2	129 original
9831	126 [559; Erythritol (4TMS)]	134 Isomaltose	45 0.220	0.581	26,285	0.679	62	79	38	103	124	4 original
16385	126 [559; Erythritol (4TMS)]	57 [757; 2-Desoxy-pentose-3-ylose dimethoxyamine (2TMS)]	45 0.212	0.556	12,985	0.654	63	78	42	99	64	17 duplicate
19571	126 [559; Erythritol (4TMS)]	116 [882; Pseudouridine (5TMS)]	20 0.211	0.908	5,921	0.567	64	77	6	135	10	64 duplicate
12048	126 [559; Erythritol (4TMS)]	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	45 0.208	0.514	18,565	0.666	65	76	58	83	104	9 duplicate
15333	126 [559; Erythritol (4TMS)]	46 Arabinose	45 0.202	0.551	18,053	0.656	66	72	44	97	100	15 duplicate
19718	126 [559; Erythritol (4TMS)]	67 [945; Galactofuranose-6-phosphate (7TMS)]	45 0.202	0.418	11,941	0.613	67	73	63	78	58	34 duplicate
17170	126 [559; Erythritol (4TMS)]	123 Citric acid	45 0.202	0.349	21,165	0.396	68	74	70	71	114	125 duplicate
19751	126 [559; Erythritol (4TMS)]	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	45 0.202	0.194	32,625	0.577	69	75	79	62	134	56 duplicate
17021	126 [559; Erythritol (4TMS)]	65 [646; 3-Deoxyglucitol (5TMS)]	45 0.200	0.612	9,074	0.656	70	70	38	105	37	14 duplicate
9836	126 [559; Erythritol (4TMS)]	139 [700; Ergosta-5,7-dien-3-ol]	26 0.200	0.305	15,054	0.308	71	71	71	70	80	138 original
19241	126 [559; Erythritol (4TMS)]	105 [705; 2-Ketogluconic acid (5TMS)]	45 0.190	0.349	13,091	0.529	72	69	69	72	67	80 duplicate
18881	126 [559; Erythritol (4TMS)]	96 myo-Inositol	31 0.174	0.185	14,584	0.230	73	68	80	61	78	139 duplicate
18483	126 [559; Erythritol (4TMS)]	88 Gluconic acid	45 0.174	0.401	13,518	0.653	74	67	64	77	70	19 duplicate
11670	126 [559; Erythritol (4TMS)]	13 Urcil	45 0.160	0.523	17,457	0.642	75	66	52	89	96	22 duplicate
12172	126 [559; Erythritol (4TMS)]	17 [700; 2-methyl-1,2-propanediol (2TMS)]	45 0.152	0.458	18,744	0.582	76	65	61	80	106	53 duplicate
16057	126 [559; Erythritol (4TMS)]	54 [NA]	45 0.149	0.356	7,384	0.585	77	64	68	73	21	52 duplicate
19168	126 [559; Erythritol (4TMS)]	103 [648; Ethylamine (2TMS)]	45 0.147	0.209	15,612	0.488	78	63	78	63	83	95 duplicate
16631	126 [559; Erythritol (4TMS)]	60 Glycerol-3-phosphate	45 0.131	0.358	18,452	0.540	79	62	66	75	103	77 duplicate
15882	126 [559; Erythritol (4TMS)]	52 [NA]	29 0.074	-0.119	16,105	0.626	80	61	105	36	88	29 duplicate
18743	126 [559; Erythritol (4TMS)]	93 [607; Putrescine (4TMS)]	44 0.057	0.002	13,527	0.350	81	60	93	48	71	133 duplicate
10753	126 [559; Erythritol (4TMS)]	6 Glycerol	45 0.051	0.085	38,635	0.594	82	59	83	58	140	42 duplicate
18925	126 [559; Erythritol (4TMS)]	97 [756; beta-D-Methylglucopyranoside (4TMS)]	45 0.040	-0.011	22,905	0.573	83	58	95	46	117	60 duplicate
10345	126 [559; Erythritol (4TMS)]	3 Ethanolamine	43 0.037	0.056	9,914	0.577	84	57	86	55	43	55 duplicate
18440	126 [559; Erythritol (4TMS)]	87 [945; beta-D-Glucopyranose (5TMS)]	43 0.034	0.231	34,640	0.586	85	56	76	65	137	50 duplicate
19091	126 [559; Erythritol (4TMS)]	101 [832; Dopamine (4TMS)]	45 0.020	0.009	13,179	0.414	86	55	91	50	68	121 duplicate
14338	126 [559; Erythritol (4TMS)]	36 [596; N-Acetylgutamic acid (2TMS)]	45 0.008	0.086	24,819	0.468	87	54	82	59	120	100 duplicate
19343	126 [559; Erythritol (4TMS)]	108 Octadecanoic acid	45 -0.006	0.011	7,983	0.439	88	53	90	51	25	113 duplicate

18275	126 [559; Erythritol (4TMS)]	84	Mannitol	43	-0.012	-0.164	30.778	0.569	89	52	107	34	130	63 duplicate
14442	126 [559; Erythritol (4TMS)]	37	Phenylalanine	45	-0.018	0.031	20.310	0.452	90	51	89	52	113	105 duplicate
9827	126 [559; Erythritol (4TMS)]	130	Trehalose	45	-0.036	-0.049	26.859	0.473	91	50	99	42	127	98 original
10887	126 [559; Erythritol (4TMS)]	7	Threonine	45	-0.042	0.058	26.673	0.339	92	49	85	58	128	136 duplicate
19010	126 [559; Erythritol (4TMS)]	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	36	-0.048	0.253	8.154	0.596	93	47	74	67	27	41 duplicate
17243	126 [559; Erythritol (4TMS)]	68	[570; Hypoxanthine (2TMS)]	7	-0.048	-0.204	11.627	0.083	94	48	109	32	55	140 duplicate
15970	126 [559; Erythritol (4TMS)]	53	Glycerol-2-phosphate	45	-0.075	-0.216	9.374	0.387	95	46	110	31	38	128 duplicate
17726	126 [559; Erythritol (4TMS)]	75	Lysine	45	-0.085	0.033	34.378	0.511	96	45	88	53	136	87 duplicate
18646	126 [559; Erythritol (4TMS)]	91	[766; beta-D-Methylglucopyranoside (4TMS)]	45	-0.089	-0.178	19.756	0.439	97	44	108	33	111	112 duplicate
18101	126 [559; Erythritol (4TMS)]	81	Tyrosine	45	-0.091	-0.009	25.567	0.669	98	43	94	47	123	8 duplicate
17980	126 [559; Erythritol (4TMS)]	79	Glucose	45	-0.097	-0.067	33.966	0.630	99	42	101	40	135	27 duplicate
16468	126 [559; Erythritol (4TMS)]	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4(E)-hydroxycyclohexane (1TMS)]	45	-0.107	0.044	15.519	0.449	100	41	87	54	82	108 duplicate
17096	126 [559; Erythritol (4TMS)]	66	Glyceric acid-3-phosphate	45	-0.115	-0.115	8.160	0.585	101	40	104	37	28	51 duplicate
11152	126 [559; Erythritol (4TMS)]	9	Proline	44	-0.123	0.008	23.002	0.419	102	39	92	49	118	120 duplicate
19818	126 [559; Erythritol (4TMS)]	118	[928; Glucopyranose-6-phosphate (6TMS)]	45	-0.127	-0.155	9.465	0.422	103	38	106	35	41	118 duplicate
17855	126 [559; Erythritol (4TMS)]	77	[826; beta-[(5-methyl-2-thienyl)methyl]eneamino-benzeneacetic acid methyl ester]	43	-0.134	-0.043	22.532	0.411	104	37	97	44	116	122 duplicate
16550	126 [559; Erythritol (4TMS)]	59	Ornithine; Arginine	45	-0.143	-0.102	34.682	0.452	105	36	103	38	138	106 duplicate
18041	126 [559; Erythritol (4TMS)]	80	[772; D-Glucose (5TMS)]	43	-0.150	-0.092	30.904	0.552	106	35	102	39	131	71 duplicate
16945	126 [559; Erythritol (4TMS)]	64	[789; Tyramine (3TMS)]	45	-0.174	-0.316	8.091	0.466	107	34	117	24	26	101 duplicate
10482	126 [559; Erythritol (4TMS)]	4	Phosphoric acid	33	-0.178	-0.066	27.586	0.420	108	33	100	41	128	119 duplicate
10207	126 [559; Erythritol (4TMS)]	2	Serine	43	-0.181	-0.043	17.480	0.442	109	32	98	43	97	110 duplicate
18836	126 [559; Erythritol (4TMS)]	95	[770; 3,4,6-Trisubhydroxyphenylethanolamine (5TMS)]	31	-0.183	-0.400	13.687	0.462	110	31	120	21	73	102 duplicate
13803	126 [559; Erythritol (4TMS)]	31	[622; Parabenic acid (2TMS)]	45	-0.194	-0.307	10.662	0.495	111	30	116	25	49	94 duplicate
18545	126 [559; Erythritol (4TMS)]	89	[775; Dopamine (4TMS)]	19	-0.205	-0.304	15.270	0.455	112	29	114	27	81	104 duplicate
13912	126 [559; Erythritol (4TMS)]	32	[729; N,N-Dimethyllysine methyl ester]	44	-0.209	-0.305	18.502	0.527	113	28	115	26	90	82 duplicate
11283	126 [559; Erythritol (4TMS)]	10	Glycine	45	-0.232	-0.577	15.719	0.661	114	27	129	12	84	111 duplicate
11020	126 [559; Erythritol (4TMS)]	8	Isoleucine	36	-0.235	-0.030	16.623	0.388	115	26	96	45	91	127 duplicate
17525	126 [559; Erythritol (4TMS)]	72	[919; D-Xylopyranose (4TMS)]	44	-0.237	-0.351	10.341	0.431	116	25	118	23	46	115 duplicate
14127	126 [559; Erythritol (4TMS)]	34	Aspartic acid	45	-0.259	-0.274	28.233	0.348	117	24	113	28	129	134 duplicate
15427	126 [559; Erythritol (4TMS)]	47	[NA]	45	-0.261	-0.457	13.605	0.632	118	23	122	19	72	26 duplicate
16868	126 [559; Erythritol (4TMS)]	63	Glutamine	35	-0.264	0.113	12.521	0.577	119	22	81	60	61	57 duplicate
14947	126 [559; Erythritol (4TMS)]	42	Glutamic acid	41	-0.266	-0.253	23.473	0.391	120	21	111	30	119	128 duplicate
11923	126 [559; Erythritol (4TMS)]	15	Alanine	45	-0.275	-0.490	20.231	0.613	121	20	124	17	112	33 duplicate
13693	126 [559; Erythritol (4TMS)]	30	[815; Ethyl-3(2H)-thiophenone]	45	-0.277	-0.254	25.217	0.334	122	19	112	29	122	137 duplicate
15520	126 [559; Erythritol (4TMS)]	48	Asparagine	45	-0.297	-0.563	11.121	0.586	123	18	128	13	50	49 duplicate
18711	126 [559; Erythritol (4TMS)]	61	[NA]	45	-0.309	-0.412	8.215	0.488	124	17	121	20	30	90 duplicate
12895	126 [559; Erythritol (4TMS)]	23	Homoserine	45	-0.311	-0.606	13.335	0.517	125	16	131	10	69	84 duplicate
14020	126 [559; Erythritol (4TMS)]	33	Methionine	45	-0.347	-0.381	12.849	0.383	126	15	119	22	63	131 duplicate
16143	126 [559; Erythritol (4TMS)]	55	[812; 4-Aminobutyric acid (2TBS)]	24	-0.348	-0.464	18.417	0.559	127	14	123	18	102	66 duplicate
13357	126 [559; Erythritol (4TMS)]	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	34	-0.365	-0.598	19.326	0.457	128	13	130	11	108	103 duplicate
17315	126 [559; Erythritol (4TMS)]	69	Arginine	41	-0.366	-0.537	17.821	0.597	129	12	126	15	98	39 duplicate
15793	126 [559; Erythritol (4TMS)]	51	[489; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	27	-0.390	-0.528	15.898	0.448	130	11	125	16	86	109 duplicate
18160	126 [559; Erythritol (4TMS)]	82	Lysine	33	-0.390	-0.774	10.429	0.575	131	10	136	5	47	59 duplicate
10068	126 [559; Erythritol (4TMS)]	1	[938; Sulfuric acid (2TMS)]	33	-0.417	-0.552	10.462	0.638	132	9	127	14	48	24 duplicate
15238	126 [559; Erythritol (4TMS)]	45	Homocysteine	42	-0.477	-0.615	17.274	0.438	133	8	132	9	94	114 duplicate
9828	126 [559; Erythritol (4TMS)]	131	[626; 5-Methylthioadenosine (3TMS)]	38	-0.525	-0.792	14.262	0.591	134	7	138	3	77	44 original
10618	126 [559; Erythritol (4TMS)]	5	Leucine	26	-0.538	-0.792	13.693	0.474	135	6	137	4	74	97 duplicate
15612	126 [559; Erythritol (4TMS)]	49	[877; Pyrophosphoric acid (4TMS)]	45	-0.539	-0.684	19.616	0.546	136	5	134	7	109	75 duplicate
15045	126 [559; Erythritol (4TMS)]	43	[548; Leucine (2TBS)]	41	-0.546	-0.645	11.479	0.373	137	4	133	8	54	132 duplicate



18968	126 [559; Erythritol (4TMS)]	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	31	-0.578	-0.811	15.776	0.497	138	3	139	2	85	91 duplicate
13128	126 [558; Erythritol (4TMS)]	25	[709; 2,5-Diaminovalerolactam (2TMS)]	42	-0.589	-0.887	17.329	0.618	139	2	135	6	95	30 duplicate
12538	127 [777; Fructose-6-phosphat	20	[618; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	13	-0.667	-0.946	13.024	0.558	140	1	140	1	65	67 duplicate
9839	127 [777; Fructose-6-phosphat	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	38	0.644	0.875	4.901	0.555	1	140	1	140	12	43 original
18332	127 [777; Fructose-6-phosphat	85	[528; Methylcitric acid (4TMS)]	23	0.494	0.822	4.215	0.401	2	139	24	117	4	89 duplicate
18696	127 [777; Fructose-6-phosphat	92	[680; Glycerol-2-phosphate (4TMS)]	39	0.471	0.545	4.854	0.581	3	138	33	108	11	33 duplicate
19052	127 [777; Fructose-6-phosphat	100	[857; Mannitol (6TMS)]	39	0.449	0.631	6.507	0.587	4	137	22	119	28	28 duplicate
19242	127 [777; Fructose-6-phosphat	105	[705; 2-Ketogluconic acid (5TMS)]	39	0.436	0.654	9.516	0.428	5	135	17	124	55	76 duplicate
19169	127 [777; Fructose-6-phosphat	103	[648; Ethylamine (2TMS)]	39	0.436	0.594	11.739	0.420	6	136	28	113	74	81 duplicate
19767	127 [777; Fructose-6-phosphat	128	[559; Erythritol (4TMS)]	39	0.401	0.515	5.849	0.452	7	134	40	101	21	67 duplicate
19466	127 [777; Fructose-6-phosphat	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	39	0.393	0.594	11.704	0.481	8	133	27	114	73	58 duplicate
19277	127 [777; Fructose-6-phosphat	108	[733; Threitol (4TMS)]	39	0.387	0.508	8.720	0.617	9	132	41	100	51	18 duplicate
16302	127 [777; Fructose-6-phosphat	56	[828; Orotic acid (3TMS)]	39	0.385	0.708	4.649	0.660	10	131	9	132	7	9 duplicate
13471	127 [777; Fructose-6-phosphat	28	Malic acid	39	0.379	0.664	7.053	0.556	11	130	16	125	31	42 duplicate
12778	127 [777; Fructose-6-phosphat	22	[690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	34	0.376	0.835	5.242	0.617	12	129	2	139	14	17 duplicate
19596	127 [777; Fructose-6-phosphat	117	[724; Glycerol (3TMS)]	39	0.374	0.560	5.246	0.504	13	126	31	110	16	53 duplicate
9846	127 [777; Fructose-6-phosphat	135												
19407	127 [777; Fructose-6-phosphat	110	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	39	0.374	0.542	8.701	0.449	14	127	34	107	50	68 original
19701	127 [777; Fructose-6-phosphat	122	[715; Erythritol (4TMS)]	39	0.374	0.534	5.832	0.605	15	128	36	105	20	22 duplicate
19547	127 [777; Fructose-6-phosphat	115	[644; Erythritol (4TMS)]	39	0.371	0.605	8.068	0.530	16	125	25	116	44	47 duplicate
9845	127 [777; Fructose-6-phosphat	134	Glucose-6-phosphate	39	0.368	0.465	21.264	0.668	17	124	45	96	123	6 duplicate
19682	127 [777; Fructose-6-phosphat	121	[657; Erythritol (4TMS)]	39	0.366	0.739	23.132	0.673	18	123	5	136	128	5 original
11798	127 [777; Fructose-6-phosphat	14	Fumaric acid	39	0.360	0.445	8.280	0.482	19	122	51	90	45	57 duplicate
19092	127 [777; Fructose-6-phosphat	101	[832; Dopamine (4TMS)]	39	0.358	0.639	5.024	0.570	20	120	20	121	13	36 duplicate
14546	127 [777; Fructose-6-phosphat	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	39	0.358	0.451	8.801	0.300	21	121	49	92	52	113 duplicate
13244	127 [777; Fructose-6-phosphat	26	Citramalic acid	39	0.352	0.711	5.902	0.665	22	119	7	134	23	7 duplicate
9847	127 [777; Fructose-6-phosphat	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	39	0.347	0.537	12.052	0.493	23	118	35	106	76	56 duplicate
16386	127 [777; Fructose-6-phosphat	57	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	17	0.338	0.465	2.882	0.369	24	117	48	95	1	99 original
19131	127 [777; Fructose-6-phosphat	102	[904; Galactose methoxyamine (5TMS)]	39	0.336	0.691	10.241	0.649	25	115	10	131	58	13 duplicate
18494	127 [777; Fructose-6-phosphat	88	Gluconic acid	39	0.336	0.505	4.476	0.583	26	116	42	99	6	31 duplicate
18826	127 [777; Fructose-6-phosphat	97	[756; beta-D-Methylglucopyranoside (4TMS)]	39	0.333	0.501	10.437	0.596	27	113	43	98	61	25 duplicate
16058	127 [777; Fructose-6-phosphat	54	[NA]	39	0.333	0.451	18.726	0.449	28	114	48	93	115	69 duplicate
18387	127 [777; Fructose-6-phosphat	86	[793; D-Galactono-1,4-lactone (4TMS)]	39	0.331	0.641	4.713	0.596	29	112	19	122	8	28 duplicate
13583	127 [777; Fructose-6-phosphat	29	Erythritol	36	0.321	0.689	19.224	0.696	30	111	11	130	116	1 duplicate
9840	127 [777; Fructose-6-phosphat	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	39	0.317	0.645	4.128	0.593	31	110	18	123	3	27 duplicate
14234	127 [777; Fructose-6-phosphat	35	Pyrogulamic acid	39	0.314	0.631	7.218	0.678	32	109	23	118	33	4 original
17022	127 [777; Fructose-6-phosphat	65	[646; 3-Deoxyglucitol (5TMS)]	39	0.301	0.335	33.439	0.641	33	108	61	80	140	14 duplicate
14648	127 [777; Fructose-6-phosphat	39	[828; 1-Phenylethanol (1TMS)]	39	0.293	0.727	6.409	0.879	34	107	6	135	27	3 duplicate
11543	127 [777; Fructose-6-phosphat	12	Glyceric acid	39	0.287	0.709	14.432	0.834	35	105	8	133	88	16 duplicate
13013	127 [777; Fructose-6-phosphat	24	[725; 2-Ketocacetic acid (2TMS)]	39	0.285	0.632	6.138	0.600	36	106	21	120	25	24 duplicate
15704	127 [777; Fructose-6-phosphat	50	[746; Ribonic acid-1,4-lactone (3TMS)]	39	0.279	0.595	11.234	0.616	37	104	12	129	133	12 duplicate
18744	127 [777; Fructose-6-phosphat	93	[607; Putrescine (4TMS)]	38	0.277	0.358	11.442	0.252	39	102	58	83	72	19 duplicate
9843	127 [777; Fructose-6-phosphat	132	[895; Isomaltose methoxyamine (8TMS)]	35	0.277	0.822	8.415	0.582	40	101	3	138	46	32 original
11671	127 [777; Fructose-6-phosphat	13	Uracil	39	0.277	0.677	14.238	0.614	41	99	14	127	85	20 duplicate
18597	127 [777; Fructose-6-phosphat	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	39	0.277	0.397	4.750	0.341	42	100	53	88	9	108 duplicate
15143	127 [777; Fructose-6-phosphat	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	39	0.271	0.497	7.750	0.538	43	98	44	97	41	45 duplicate
12049	127 [777; Fructose-6-phosphat	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	39	0.266	0.673	14.994	0.636	44	96	15	126	92	15 duplicate

19311	127 [777]; Fructose-6-phosph	107	9-(Z)-Octadecenoic acid	39	0.266	0.275	9.434	0.396	45	97	68	73	54	91 duplicate
11414	127 [777]; Fructose-6-phosph	11	Succinic acid	39	0.263	0.563	6.022	0.586	46	95	30	111	24	30 duplicate
15334	127 [777]; Fructose-6-phosph	46	Arabinose	39	0.258	0.677	15.153	0.684	47	93	13	128	93	2 duplicate
14749	127 [777]; Fructose-6-phosph	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	39	0.258	0.456	26.547	0.496	48	94	47	94	132	55 duplicate
19641	127 [777]; Fructose-6-phosph	119	[931; myo-Inositol-2-phosphate (7TMS)]	39	0.255	0.448	4.768	0.471	49	92	50	91	10	61 duplicate
19572	127 [777]; Fructose-6-phosph	116	[882; Pseudouridine (5TMS)]	39	0.255	0.754	3.806	0.470	50	91	4	137	2	62 duplicate
16791	127 [777]; Fructose-6-phosph	62	[912; D-Xylofuranose (4TMS)]	39	0.250	0.522	11.250	0.665	51	90	38	103	70	83 duplicate
18647	127 [777]; Fructose-6-phosph	91	[766; beta-D-Methylglucopyranoside (4TMS)]	39	0.236	0.393	14.874	0.271	52	89	55	86	91	120 duplicate
15883	127 [777]; Fructose-6-phosph	52	[NA]	28	0.233	0.375	17.320	0.477	53	88	58	85	108	60 duplicate
17594	127 [777]; Fructose-6-phosph	73	[708; Glucose methoxyamine (5TMS)]	32	0.218	0.295	6.649	0.391	54	87	65	76	29	95 duplicate
9852	127 [777]; Fructose-6-phosph	141	Lanosta-8,24-dien-3-beta-ol	36	0.210	0.311	9.612	0.443	55	86	63	78	56	71 original
12659	127 [777]; Fructose-6-phosph	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	39	0.209	0.384	13.058	0.468	56	85	54	87	82	63 duplicate
18441	127 [777]; Fructose-6-phosph	87	[945; beta-D-Glucopyranose (5TMS)]	37	0.204	0.525	28.124	0.587	57	84	37	104	138	29 duplicate
17792	127 [777]; Fructose-6-phosph	76	Fructose	39	0.190	0.438	22.903	0.609	58	83	52	89	127	21 duplicate
9851	127 [777]; Fructose-6-phosph	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	29	0.187	0.355	10.987	0.440	59	82	59	82	67	72 original
12173	127 [777]; Fructose-6-phosph	17	[700; 2-methyl-1,2-propanediol (2TMS)]	39	0.185	0.593	15.226	0.575	60	81	29	112	94	35 duplicate
18791	127 [777]; Fructose-6-phosph	94	Hexadecanoic acid	39	0.179	0.291	17.245	0.344	61	80	66	75	107	104 duplicate
14849	127 [777]; Fructose-6-phosph	41	[639; Proline (2TMS)]	39	0.171	0.280	10.388	0.422	62	79	67	74	59	80 duplicate
17387	127 [777]; Fructose-6-phosph	70	[893; 2-Furan-2-hydroxyacetic acid (2TMS)]	33	0.170	0.053	15.585	0.447	63	78	84	57	99	70 duplicate
17661	127 [777]; Fructose-6-phosph	74	[912; Tetradecanoic acid (1TMS)]	39	0.163	0.366	7.701	0.294	64	76	57	84	40	117 duplicate
12296	127 [777]; Fructose-6-phosph	18	[590; 1-Acetyl-2-thiohydantoin]	39	0.163	0.234	6.149	0.358	65	77	72	69	28	101 duplicate
19011	127 [777]; Fructose-6-phosph	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	33	0.155	0.520	5.274	0.604	66	75	39	102	17	23 duplicate
19376	127 [777]; Fructose-6-phosph	109	Octadecanoic acid	39	0.147	0.273	19.587	0.372	67	74	69	72	119	98 duplicate
9850	127 [777]; Fructose-6-phosph	139	[700; Ergosta-5,7-dien-3-ol]	25	0.147	0.322	14.673	0.429	68	73	62	79	89	77 original
19662	127 [777]; Fructose-6-phosph	120	[945; Uridine (3TMS)]	38	0.147	-0.023	10.434	0.521	69	72	88	53	60	50 duplicate
17526	127 [777]; Fructose-6-phosph	72	[919; D-Xylopyranose (4TMS)]	38	0.141	0.185	7.354	0.335	70	71	75	66	35	109 duplicate
16869	127 [777]; Fructose-6-phosph	63	Glutamine	34	0.137	0.559	12.124	0.653	71	70	32	109	77	11 duplicate
18219	127 [777]; Fructose-6-phosph	83	Sorbitol	33	0.136	-0.143	15.801	0.132	72	69	97	44	100	137 duplicate
18276	127 [777]; Fructose-6-phosph	84	Mannitol	37	0.132	0.345	25.981	0.411	73	68	60	81	131	83 duplicate
12418	127 [777]; Fructose-6-phosph	19	Alanine (BP) (3TMS)	39	0.131	0.230	9.690	0.426	74	67	73	68	57	79 duplicate
19437	127 [777]; Fructose-6-phosph	111	[583; Erythritol (4TMS)]	32	0.125	0.146	16.268	0.400	75	66	76	65	103	90 duplicate
9848	127 [777]; Fructose-6-phosph	137	Ergosterol	39	0.112	0.053	11.061	0.377	76	65	85	56	68	97 original
15428	127 [777]; Fructose-6-phosph	47	[NA]	39	0.104	0.300	7.767	0.499	77	64	64	77	42	54 duplicate
18042	127 [777]; Fructose-6-phosph	80	[772; D-Glucose (5TMS)]	37	0.090	0.261	24.724	0.523	78	63	70	71	130	49 duplicate
17919	127 [777]; Fructose-6-phosph	78	Mannose	37	0.081	0.235	5.870	0.581	79	62	71	70	22	34 duplicate
19521	127 [777]; Fructose-6-phosph	114	Fructose-6-phosphate	37	0.066	0.059	4.466	0.562	80	61	83	58	5	41 duplicate
19494	127 [777]; Fructose-6-phosph	113	Galactose-6-phosphate	39	0.058	0.080	5.243	0.568	81	60	81	60	15	38 duplicate
9849	127 [777]; Fructose-6-phosph	138	[674; Ergosterol (1TMS)]	30	0.057	0.100	12.700	0.368	82	59	80	61	80	100 original
18882	127 [777]; Fructose-6-phosph	96	myo-Inositol	27	0.048	0.207	13.948	0.313	83	58	74	67	83	111 duplicate
19719	127 [777]; Fructose-6-phosph	123	[945; Galactofuranose-6-phosphate (7TMS)]	39	0.047	-0.076	8.628	0.459	84	57	93	48	48	65 duplicate
18546	127 [777]; Fructose-6-phosph	89	[775; Dopamine (4TMS)]	18	0.046	0.110	14.478	0.353	85	56	79	62	87	102 duplicate
19736	127 [777]; Fructose-6-phosph	124	[734; 1-Monoleoylglycerol (2TMS); 1-Monohexadecyloxyglycerol (1TMS)]	35	0.045	0.119	18.388	0.426	86	55	78	63	112	78 duplicate
9844	127 [777]; Fructose-6-phosph	133	[855; Squalene]	39	0.036	-0.027	7.559	0.278	87	54	89	52	38	118 original
15971	127 [777]; Fructose-6-phosph	53	Glycerol-2-phosphate	39	0.034	0.020	8.801	0.294	88	53	86	55	53	116 duplicate
17457	127 [777]; Fructose-6-phosph	71	[731; Erythrose (3TMS)]	39	0.028	-0.037	8.567	0.344	89	52	90	51	47	105 duplicate
19206	127 [777]; Fructose-6-phosph	104	[785; Erythritol (4TMS)]	38	-0.010	-0.014	7.242	0.402	90	51	87	54	34	85 duplicate
10069	127 [777]; Fructose-6-phosph	1	[936; Sulfuric acid (2TMS)]	33	-0.011	0.121	7.073	0.520	91	50	77	64	32	51 duplicate
19619	127 [777]; Fructose-6-phosph	118	[928; Glucopyranose-6-phosphate (6TMS)]	39	-0.023	0.072	6.652	0.411	92	49	82	59	30	84 duplicate
19752	127 [777]; Fructose-6-phosph	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	39	-0.034	-0.083	27.701	0.567	93	48	94	47	134	39 duplicate
17171	127 [777]; Fructose-6-phosph	67	Citric acid	39	-0.050	-0.153	18.882	0.272	94	47	98	43	105	119 duplicate

18837	127	[777]	Fructose-6-phosph	95	[770; 3,4,6-Trisubstituted phenylethanolamine (5TMS)]	25	-0.060	-0.101	15,411	0.261	95	46	95	46	96	122	duplicate
15239	127	[777]	Fructose-6-phosph	45	Homocysteine	36	-0.067	-0.178	17,762	0.342	96	45	101	40	110	107	duplicate
16632	127	[777]	Fructose-6-phosph	60	Glycerol-3-phosphate	39	-0.072	-0.074	14,613	0.353	97	44	92	49	88	103	duplicate
15613	127	[777]	Fructose-6-phosph	49	[877; Pyrophosphoric acid (4TMS)]	39	-0.074	-0.106	18,701	0.393	98	43	96	45	114	83	duplicate
18344	127	[777]	Fructose-6-phosph	108	Octadecenoic acid	39	-0.077	-0.168	7,406	0.401	99	42	100	41	36	87	duplicate
1414128	127	[777]	Fructose-6-phosph	34	Aspartic acid	39	-0.085	-0.251	22,547	0.249	100	41	104	37	128	128	duplicate
13694	127	[777]	Fructose-6-phosph	30	[815; Ethyl-3(2H)-thiophenone]	39	-0.093	-0.305	19,687	0.176	101	40	111	30	120	133	duplicate
17856	127	[777]	Fructose-6-phosph	77	benzeneacetic acid methyl ester]	37	-0.096	-0.267	18,122	0.269	102	39	105	36	111	121	duplicate
10754	127	[777]	Fructose-6-phosph	6	Glycerol	39	-0.101	-0.044	33,003	0.528	103	38	91	50	139	48	duplicate
14443	127	[777]	Fructose-6-phosph	37	Phenylalanine	39	-0.104	-0.292	15,920	0.307	104	37	109	32	101	112	duplicate
171316	127	[777]	Fructose-6-phosph	69	Arginine	35	-0.106	-0.495	12,776	0.536	105	36	128	13	81	46	duplicate
16551	127	[777]	Fructose-6-phosph	59	Omithine; Arginine	39	-0.131	-0.302	29,028	0.300	106	35	110	31	137	114	duplicate
14021	127	[777]	Fructose-6-phosph	33	Methionine	39	-0.134	-0.337	10,534	0.247	107	34	113	28	62	127	duplicate
16712	127	[777]	Fructose-6-phosph	61	[NA]	39	-0.152	-0.233	5,458	0.454	108	33	102	39	18	68	duplicate
15521	127	[777]	Fructose-6-phosph	48	Asparagine	39	-0.158	-0.276	8,679	0.569	109	32	107	34	49	37	duplicate
15046	127	[777]	Fructose-6-phosph	43	[548; Leucine (2TBS)]	35	-0.187	-0.251	7,619	0.299	110	31	103	38	39	115	duplicate
13913	127	[777]	Fructose-6-phosph	32	[729; N,N-Dimethyllysine methyl ester]	38	-0.188	-0.482	16,996	0.380	111	30	126	15	106	98	duplicate
14948	127	[777]	Fructose-6-phosph	42	Glutamic acid	35	-0.200	-0.436	18,442	0.185	112	29	124	17	113	132	duplicate
10888	127	[777]	Fructose-6-phosph	7	Threonine	39	-0.201	-0.324	21,860	0.185	113	28	112	29	125	131	duplicate
18161	127	[777]	Fructose-6-phosph	82	Lysine	19	-0.205	-0.483	8,045	0.392	114	27	127	14	43	94	duplicate
11924	127	[777]	Fructose-6-phosph	15	Alanine	39	-0.212	-0.564	15,228	0.563	115	26	132	9	95	40	duplicate
9841	127	[777]	Fructose-6-phosph	130	Trehalose	39	-0.217	-0.360	21,834	0.429	116	25	116	25	124	75	original
10346	127	[777]	Fructose-6-phosph	3	Ethanolamine	37	-0.222	-0.376	10,884	0.463	117	24	119	22	64	64	duplicate
16946	127	[777]	Fructose-6-phosph	64	[789; Tyramine (3TMS)]	39	-0.228	-0.434	5,652	0.434	118	23	123	18	19	74	duplicate
16469	127	[777]	Fructose-6-phosph	58	[836; 4R-Acetanilido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	39	-0.233	-0.291	12,176	0.194	119	21	108	33	78	130	duplicate
18102	127	[777]	Fructose-6-phosph	81	Tyrosine	39	-0.233	-0.386	20,716	0.479	120	22	120	21	122	59	duplicate
17244	127	[777]	Fructose-6-phosph	68	[570; Hypoxanthine (2TMS)]	7	-0.238	-0.157	12,561	0.002	121	20	99	42	79	140	duplicate
14339	127	[777]	Fructose-6-phosph	36	[596; N-Acetylglutamic acid (2TMS)]	39	-0.244	-0.364	20,294	0.218	122	19	118	23	121	128	duplicate
11153	127	[777]	Fructose-6-phosph	9	Proline	38	-0.246	-0.356	19,465	0.156	123	18	115	26	118	134	duplicate
171727	127	[777]	Fructose-6-phosph	75	Lysine	39	-0.247	-0.361	28,855	0.250	124	17	117	24	136	125	duplicate
11264	127	[777]	Fructose-6-phosph	10	Glycine	39	-0.250	-0.643	10,954	0.654	125	16	136	5	68	10	duplicate
13804	127	[777]	Fructose-6-phosph	31	[622; Parabanic acid (2TMS)]	39	-0.285	-0.519	10,941	0.440	126	15	131	10	65	73	duplicate
10208	127	[777]	Fructose-6-phosph	2	Serine	37	-0.285	-0.395	15,414	0.149	127	14	121	20	97	135	duplicate
11021	127	[777]	Fructose-6-phosph	8	Isoleucine	30	-0.297	-0.274	14,692	0.061	128	13	106	35	90	139	duplicate
17097	127	[777]	Fructose-6-phosph	66	Glyceric acid-3-phosphate	39	-0.301	-0.513	7,536	0.394	129	12	129	12	37	92	duplicate
13129	127	[777]	Fructose-6-phosph	25	[709; 2,5-Diaminovalerolactam (2TMS)]	36	-0.311	-0.740	15,418	0.543	130	11	139	2	98	44	duplicate
13358	127	[777]	Fructose-6-phosph	27	[815; (E)-4-Methyl-5-hydroxy-3-pentan-2-one (1TMS)]	28	-0.312	-0.618	19,412	0.253	131	10	135	6	117	123	duplicate
15794	127	[777]	Fructose-6-phosph	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	21	-0.314	-0.467	16,258	0.214	132	9	125	16	102	129	duplicate
12896	127	[777]	Fructose-6-phosph	23	Homoserine	39	-0.325	-0.654	10,687	0.401	133	8	137	4	63	88	duplicate
17981	127	[777]	Fructose-6-phosph	79	Glucose	39	-0.344	-0.518	28,587	0.519	134	7	130	11	135	52	duplicate
10483	127	[777]	Fructose-6-phosph	4	Phosphoric acid	27	-0.362	-0.342	23,498	0.136	135	6	114	27	129	136	duplicate
9842	127	[777]	Fructose-6-phosph	131	[626; 5-Methylthioadenosine (3TMS)]	32	-0.395	-0.402	14,237	0.401	136	5	122	19	84	88	original
16144	127	[777]	Fructose-6-phosph	55	[612; 4-Aminobutyric acid (2TBS)]	18	-0.399	-0.613	16,469	0.417	137	4	134	7	104	82	duplicate
12539	127	[777]	Fructose-6-phosph	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	10	-0.467	-0.889	11,947	0.343	138	3	140	1	75	106	duplicate
18969	127	[777]	Fructose-6-phosph	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	25	-0.480	-0.701	17,549	0.326	139	2	138	3	109	110	duplicate
10619	127	[777]	Fructose-6-phosph	5	Leucine	21	-0.524	-0.580	11,269	0.075	140	1	133	8	71	136	duplicate
19782	128	[824; D-Sedoheptulose-9]	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	38	0.644	0.875	4,901	0.555	1	140	3	138	7	40	duplicate	
18697	128	[824; D-Sedoheptulose-9]	127	[777; Glycerol-2-phosphate (4TMS)]	45	0.634	0.853	4,438	0.582	2	139	7	134	3	22	duplicate	

9858	128 [824; D-Sedoheptulose-134 Isomaltose	45	0.584	0.879	19,503	0.651	3	138	1	140	107	4 original
18333	128 [824; D-Sedoheptulose-85 [529; Methylcitric acid (4TMS)]	29	0.571	0.701	4,994	0.388	4	137	34	107	8	98 duplicate
19243	128 [824; D-Sedoheptulose-105 [705; 2-Ketoglucuronic acid (5TMS)]	44	0.564	0.824	6,459	0.528	5	136	14	127	14	51 duplicate
19170	128 [824; D-Sedoheptulose-103 [648; Ethylamine (2TMS)]	44	0.556	0.771	8,023	0.515	6	135	22	119	30	57 duplicate
16303	128 [824; D-Sedoheptulose-56 [829; Orlic acid (3TMS)]	45	0.535	0.861	3,938	0.645	7	134	6	135	1	6 duplicate
17023	128 [824; D-Sedoheptulose-65 [646; 3-Deoxyglucitol (5TMS)]	45	0.517	0.867	4,033	0.642	8	133	4	137	2	7 duplicate
16387	128 [824; D-Sedoheptulose-57 [757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	44	0.514	0.829	6,151	0.647	9	132	12	128	12	5 duplicate
15335	128 [824; D-Sedoheptulose-46 Arabinose	45	0.509	0.876	10,979	0.631	10	131	2	139	59	10 duplicate
9853	128 [824; D-Sedoheptulose-129 [840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	44	0.507	0.806	4,474	0.658	11	129	16	125	4	2 original
18927	128 [824; D-Sedoheptulose-97 [756; beta-D-Methylglucopyranoside (4TMS)]	44	0.507	0.675	14,764	0.517	12	130	37	104	83	56 duplicate
13594	128 [824; D-Sedoheptulose-29 Erythritol	45	0.499	0.838	6,159	0.566	13	128	10	131	13	34 duplicate
13014	128 [824; D-Sedoheptulose-24 [725; 2-Ketooctanoic acid (2TMS)]	45	0.493	0.846	24,799	0.633	14	128	9	132	131	9 duplicate
18495	128 [824; D-Sedoheptulose-88 Gluconic acid	45	0.493	0.689	7,482	0.593	15	127	35	108	25	17 duplicate
11672	128 [824; D-Sedoheptulose-13 Uracl	45	0.487	0.816	10,908	0.581	16	125	15	128	57	23 duplicate
14547	128 [824; D-Sedoheptulose-38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	45	0.483	0.850	4,733	0.625	17	123	8	133	5	11 duplicate
16059	128 [824; D-Sedoheptulose-54 [NA]	45	0.483	0.798	8,238	0.572	18	124	18	123	31	30 duplicate
15705	128 [824; D-Sedoheptulose-50 [746; Ribonic acid-1,4-lactone (3TMS)]	44	0.465	0.783	16,133	0.574	19	122	20	121	84	29 duplicate
14649	128 [824; D-Sedoheptulose-39 [829; 1-Phenylethanol (1TMS)]	45	0.465	0.828	10,465	0.578	20	121	13	128	52	26 duplicate
18388	128 [824; D-Sedoheptulose-86 [793; D-Galactono-1,4-lactone (4TMS)]	42	0.461	0.865	15,449	0.651	21	120	5	136	88	3 duplicate
12050	128 [824; D-Sedoheptulose-16 [644; 2-Methyl-1,3-butanediol (2TMS)]	45	0.461	0.831	12,101	0.600	22	119	11	130	64	16 duplicate
19093	128 [824; D-Sedoheptulose-101 [832; Dopamine (4TMS)]	45	0.455	0.627	6,882	0.381	23	118	41	100	19	110 duplicate
19497	128 [824; D-Sedoheptulose-112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	45	0.451	0.660	16,427	0.447	24	117	38	103	96	74 duplicate
16745	128 [824; D-Sedoheptulose-93 [607; Putrescine (4TMS)]	44	0.438	0.538	15,465	0.323	25	116	51	90	90	122 duplicate
11799	128 [824; D-Sedoheptulose-135 Fumaric acid	45	0.432	0.743	9,025	0.519	26	115	28	113	40	54 duplicate
9859	128 [824; D-Sedoheptulose-1902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	45	0.430	0.622	7,863	0.439	27	114	42	99	28	77 original
19548	128 [824; D-Sedoheptulose-115 Glucose-6-phosphate	45	0.420	0.705	19,116	0.659	28	113	33	108	105	1 duplicate
19012	128 [824; D-Sedoheptulose-99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	38	0.416	0.778	9,737	0.583	29	112	21	120	47	21 duplicate
19053	128 [824; D-Sedoheptulose-100 [857; Mannitol (5TMS)]	45	0.414	0.760	5,527	0.563	30	111	23	118	9	35 duplicate
12779	128 [824; D-Sedoheptulose-22 [690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	39	0.409	0.801	9,808	0.607	31	110	17	124	48	15 duplicate
11415	128 [824; D-Sedoheptulose-11 Succinic acid	45	0.406	0.749	5,637	0.555	32	108	26	115	10	39 duplicate
13472	128 [824; D-Sedoheptulose-28 Malic acid	45	0.406	0.748	6,074	0.522	33	109	27	114	11	53 duplicate
16792	128 [824; D-Sedoheptulose-62 [812; D-Xylofuranose (4TMS)]	45	0.404	0.751	9,485	0.634	34	107	25	116	45	8 duplicate
11544	128 [824; D-Sedoheptulose-12 Glycic acid	45	0.402	0.743	10,516	0.559	35	108	29	112	53	37 duplicate
19132	128 [824; D-Sedoheptulose-102 [904; Galactose methoxyamine (5TMS)]	45	0.390	0.714	7,599	0.522	36	105	31	110	26	52 duplicate
19408	128 [824; D-Sedoheptulose-106 [733; Threitol (4TMS)]	44	0.385	0.615	6,598	0.588	37	104	43	98	15	18 duplicate
14235	128 [824; D-Sedoheptulose-35 Pyroglycamic acid	45	0.372	0.751	32,222	0.566	39	102	24	117	139	33 duplicate
18648	128 [824; D-Sedoheptulose-91 [766; beta-D-Methylglucopyranoside (4TMS)]	45	0.370	0.544	12,498	0.382	40	101	50	91	66	103 duplicate
19702	128 [824; D-Sedoheptulose-122 [644; Erythritol (4TMS)]	44	0.368	0.657	13,037	0.538	41	100	39	102	72	45 duplicate
12174	128 [824; D-Sedoheptulose-17 [700; 2-methyl-1,2-propanediol (2TMS)]	45	0.360	0.784	12,109	0.541	42	99	19	122	65	44 duplicate
19597	128 [824; D-Sedoheptulose-117 [724; Glycerol (3TMS)]	43	0.353	0.560	6,681	0.509	43	97	48	93	16	59 duplicate
19768	128 [824; D-Sedoheptulose-126 [559; Erythritol (4TMS)]	43	0.353	0.526	8,985	0.496	44	98	52	89	39	64 duplicate
18277	128 [824; D-Sedoheptulose-84 Mannitol	43	0.344	0.551	23,315	0.441	45	96	49	92	129	76 duplicate
18598	128 [824; D-Sedoheptulose-90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	45	0.337	0.287	7,431	0.360	46	95	64	77	24	112 duplicate
17793	128 [824; D-Sedoheptulose-76 Fructose	45	0.333	0.716	20,186	0.572	47	92	30	111	112	31 duplicate
19642	128 [824; D-Sedoheptulose-119 [931; myo-Inositol-2-phosphate (7TMS)]	45	0.333	0.339	7,628	0.434	48	93	61	80	27	80 duplicate
17245	128 [824; D-Sedoheptulose-68 [570; Hypoxanthine (2TMS)]	7	0.333	0.315	15,041	0.165	49	94	62	79	85	139 duplicate
14750	128 [824; D-Sedoheptulose-40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	45	0.323	0.633	25,376	0.463	50	91	40	101	133	72 duplicate

15144	128 [824; D-Sedoheptulose-44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	44	0.307	0.563	6.945	0.537	51	90	47	94	18	47 duplicate
13245	128 [824; D-Sedoheptulose-26	Citramalic acid	45	0.305	0.575	10.763	0.492	52	89	46	95	55	68 duplicate
19663	128 [824; D-Sedoheptulose-121	[657; Erythritol (4TMS)]	42	0.292	0.398	12.676	0.512	53	88	59	82	69	58 duplicate
17920	128 [824; D-Sedoheptulose-78	Mannose	43	0.291	0.578	6.715	0.549	54	87	45	96	17	41 duplicate
9856	128 [824; D-Sedoheptulose-132	[895; Isomaltose methoxyamine (8TMS)]	37	0.285	0.709	12.655	0.579	55	86	32	108	68	25 original
15894	128 [824; D-Sedoheptulose-52	[NA]	30	0.283	0.035	22.105	0.568	56	85	81	60	124	32 duplicate
17388	128 [824; D-Sedoheptulose-70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	38	0.280	0.181	14.192	0.496	57	84	70	71	78	65 duplicate
12660	128 [824; D-Sedoheptulose-21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	45	0.267	0.454	11.360	0.503	58	83	54	87	60	61 duplicate
19573	128 [824; D-Sedoheptulose-116	[882; Pseudouridine (5TMS)]	19	0.263	0.683	6.904	0.448	59	82	36	105	20	75 duplicate
19663	128 [824; D-Sedoheptulose-130	[945; Uridine (3TMS)]	43	0.258	0.047	6.792	0.533	60	81	78	63	37	49 duplicate
9860	128 [824; D-Sedoheptulose-107	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.250	0.447	4.744	0.452	61	80	56	85	6	73 original
19312	128 [824; D-Sedoheptulose-107	9-(2)-Octadecenoic acid	45	0.244	0.067	9.262	0.402	62	79	76	65	42	88 duplicate
16870	128 [824; D-Sedoheptulose-63	Glutamine	36	0.232	-0.014	17.120	0.621	63	78	84	57	98	13 duplicate
17595	128 [824; D-Sedoheptulose-73	[708; Glucose methoxyamine (5TMS)]	38	0.223	0.492	7.160	0.410	64	77	53	88	22	85 duplicate
9865	128 [824; D-Sedoheptulose-141	Lenosta-8,24-dien-3-beta-ol	42	0.208	0.285	14.370	0.405	65	76	63	78	79	88 original
17682	128 [824; D-Sedoheptulose-74	[912; Tetradecanoic acid (1TMS)]	45	0.192	0.347	9.484	0.317	66	75	60	81	44	125 duplicate
18442	128 [824; D-Sedoheptulose-87	[945; beta-D-Glucopyranose (5TMS)]	43	0.165	0.437	28.846	0.577	67	74	57	84	136	27 duplicate
12297	128 [824; D-Sedoheptulose-18	[590; 1-Acetyl-2-thiohydantoin]	45	0.147	0.235	7.063	0.388	68	73	66	75	21	99 duplicate
18792	128 [824; D-Sedoheptulose-94	Hexadecanoic acid	45	0.143	0.207	15.774	0.388	69	72	69	72	91	97 duplicate
18753	128 [824; D-Sedoheptulose-125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	45	0.135	0.447	26.045	0.538	70	71	55	86	134	48 duplicate
18377	128 [824; D-Sedoheptulose-109	Octadecanoic acid	45	0.137	0.217	17.949	0.397	71	70	68	73	102	90 duplicate
18547	128 [824; D-Sedoheptulose-89	[775; Dopamine (4TMS)]	19	0.135	-0.396	17.838	0.390	72	69	108	33	100	95 duplicate
19438	128 [824; D-Sedoheptulose-111	[583; Erythritol (4TMS)]	35	0.119	0.253	20.637	0.381	73	68	65	76	113	104 duplicate
19495	128 [824; D-Sedoheptulose-113	Galactose-6-phosphate	45	0.109	0.431	7.303	0.576	74	67	58	83	23	28 duplicate
10070	128 [824; D-Sedoheptulose-1	[938; Sulfuric acid (2TMS)]	33	0.102	0.219	9.318	0.557	75	66	67	74	43	38 duplicate
9864	128 [824; D-Sedoheptulose-140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	31	0.097	0.156	15.025	0.379	76	65	71	70	84	105 original
15972	128 [824; D-Sedoheptulose-53	Glycerol-2-phosphate	45	0.085	0.032	12.955	0.330	77	64	82	59	71	121 duplicate
15429	128 [824; D-Sedoheptulose-47	[NA]	45	0.075	0.042	10.444	0.498	78	63	78	62	51	63 duplicate
9861	128 [824; D-Sedoheptulose-137	Ergosterol	45	0.065	-0.031	11.645	0.376	79	62	85	56	82	107 original
19737	128 [824; D-Sedoheptulose-124	[734; 1-Monooctylethylglycerol (2TMS); 1-Monohexadecenoylethylglycerol (1TMS)]	40	0.062	-0.103	23.194	0.480	80	61	88	53	128	68 duplicate
18220	128 [824; D-Sedoheptulose-83	Sorbitol	39	0.061	-0.229	16.122	0.232	81	60	99	42	93	135 duplicate
9863	128 [824; D-Sedoheptulose-139	[700; Ergosta-5,7-dien-3-ol]	27	0.043	-0.112	16.546	0.390	82	59	89	52	104	98 original
18883	128 [824; D-Sedoheptulose-96	myo-Inositol	31	0.024	0.062	17.899	0.221	83	58	77	64	101	136 duplicate
18207	128 [824; D-Sedoheptulose-104	[795; Erythritol (4TMS)]	44	0.021	0.041	8.508	0.422	84	57	80	61	35	82 duplicate
17458	128 [824; D-Sedoheptulose-71	[731; Erythrose (3TMS)]	45	0.008	-0.038	8.453	0.385	85	56	86	55	34	102 duplicate
18838	128 [824; D-Sedoheptulose-95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	31	0.006	-0.175	19.602	0.341	86	55	95	46	108	116 duplicate
14850	128 [824; D-Sedoheptulose-41	[639; Proline (3TMS)]	45	-0.002	0.086	10.108	0.437	87	54	75	68	50	78 duplicate
12419	128 [824; D-Sedoheptulose-19	Alanine (BP) (3TMS)	45	-0.006	0.153	9.246	0.518	88	53	72	69	41	55 duplicate
18043	128 [824; D-Sedoheptulose-80	[772; D-Glucose (5TMS)]	43	-0.012	0.150	24.772	0.541	89	52	73	68	130	42 duplicate
19522	128 [824; D-Sedoheptulose-114	Fructose-6-phosphate	40	-0.038	0.002	8.433	0.585	90	51	83	58	33	19 duplicate
9865	128 [824; D-Sedoheptulose-138	[674; Ergosterol (1TMS)]	31	-0.049	-0.072	16.686	0.386	91	50	87	54	97	100 original
10755	128 [824; D-Sedoheptulose-6	Glycerol	45	-0.061	0.120	32.593	0.538	92	49	74	67	140	46 duplicate
9857	128 [824; D-Sedoheptulose-133	[855; Squalene]	45	-0.089	-0.151	9.958	0.337	93	48	93	48	49	119 original
19720	128 [824; D-Sedoheptulose-123	[945; Galactofuranose-6-phosphate (7TMS)]	45	-0.089	-0.133	8.793	0.473	94	47	91	50	38	71 duplicate
17527	128 [824; D-Sedoheptulose-72	[918; D-Xylopyranose (4TMS)]	44	-0.099	-0.290	11.804	0.361	95	46	101	40	63	111 duplicate
17172	128 [824; D-Sedoheptulose-67	Citric acid	45	-0.111	-0.227	16.006	0.304	96	45	98	43	92	126 duplicate
15614	128 [824; D-Sedoheptulose-49	[877; Pyrophosphoric acid (4TMS)]	45	-0.115	-0.171	22.584	0.390	97	44	94	47	125	94 duplicate
15240	128 [824; D-Sedoheptulose-45	Homocysteine	42	-0.127	-0.181	22.083	0.346	98	43	96	45	123	114 duplicate
19345	128 [824; D-Sedoheptulose-108	Octadecenoic acid	45	-0.139	-0.325	11.390	0.378	99	42	105	36	61	106 duplicate
16713	128 [824; D-Sedoheptulose-61	[NA]	45	-0.141	-0.205	8.512	0.474	100	41	97	44	36	70 duplicate

16633	128 [824; D-Sedoheptulose-60	Glycerol-3-phosphate	45	-0.200	-0.252	14,139	0.404	101	40	100	41	77	87 duplicate
16620	128 [824; D-Sedoheptulose-118	[928; Glucopyranose-6-phosphate (6TMS)]	44	-0.211	-0.429	10,665	0.488	102	39	111	30	54	67 duplicate
15047	128 [824; D-Sedoheptulose-43	[548; Leucine (2TBS)]	41	-0.232	-0.297	9,720	0.278	103	38	102	39	46	130 duplicate
16947	128 [824; D-Sedoheptulose-84	[789; Tyramine (3TMS)]	45	-0.236	-0.139	8,424	0.435	104	37	92	49	32	79 duplicate
13130	128 [824; D-Sedoheptulose-25	[709; 2,5-Diaminovalerolactam (2TMS)]	42	-0.245	-0.714	19,617	0.528	105	36	137	4	109	50 duplicate
14129	128 [824; D-Sedoheptulose-34	Aspartic acid	45	-0.248	-0.322	22,743	0.323	106	35	104	37	127	123 duplicate
14444	128 [824; D-Sedoheptulose-37	Phenylalanine	45	-0.253	-0.410	15,346	0.413	107	34	109	32	87	84 duplicate
15795	128 [824; D-Sedoheptulose-51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	27	-0.271	-0.497	19,334	0.294	108	33	120	21	106	128 duplicate
15522	128 [824; D-Sedoheptulose-48	Asparagine	45	-0.275	-0.504	12,695	0.561	109	32	122	19	70	36 duplicate
10889	128 [824; D-Sedoheptulose-7	Threonine	45	-0.277	-0.368	21,334	0.247	110	31	107	34	118	134 duplicate
17857	128 [824; D-Sedoheptulose-77	benzeneacetic acid methyl ester]	43	-0.289	-0.477	19,996	0.279	111	30	118	23	110	129 duplicate
17317	128 [824; D-Sedoheptulose-69	Arginine	41	-0.298	-0.604	15,454	0.474	112	29	130	11	89	69 duplicate
13695	128 [824; D-Sedoheptulose-30	[815; Ethyl-3(2H)-thiophenone]	45	-0.301	-0.454	20,952	0.296	113	28	113	28	116	127 duplicate
14022	128 [824; D-Sedoheptulose-33	Methionine	45	-0.303	-0.431	13,543	0.354	114	27	112	29	74	113 duplicate
10347	128 [824; D-Sedoheptulose-3	Ethanolamine	43	-0.309	-0.465	15,169	0.504	115	26	114	27	86	60 duplicate
9854	128 [824; D-Sedoheptulose-130	Trehalose	45	-0.321	-0.515	21,622	0.416	116	25	123	18	121	83 original
11022	128 [824; D-Sedoheptulose-8	Isoleucine	36	-0.333	-0.364	16,345	0.174	117	23	106	35	95	138 duplicate
18162	128 [824; D-Sedoheptulose-82	Lysine	22	-0.333	-0.123	27,929	0.584	119	22	90	51	135	91 duplicate
17982	128 [824; D-Sedoheptulose-79	Glucose	45	-0.337	-0.123	27,929	0.584	119	22	90	51	135	20 duplicate
11925	128 [824; D-Sedoheptulose-15	Alanine	45	-0.341	-0.318	14,713	0.580	120	21	103	38	81	24 duplicate
16552	128 [824; D-Sedoheptulose-59	Ornithine; Arginine	45	-0.349	-0.475	29,512	0.340	121	20	117	24	138	117 duplicate
12897	128 [824; D-Sedoheptulose-23	Homoserine	45	-0.352	-0.664	14,011	0.425	122	19	135	6	76	81 duplicate
11154	128 [824; D-Sedoheptulose-9	Proline	44	-0.355	-0.480	21,579	0.260	123	18	119	22	119	131 duplicate
14340	128 [824; D-Sedoheptulose-38	[596; N-Acetylglutamic acid (2TMS)]	45	-0.360	-0.526	20,795	0.372	124	17	125	16	114	108 duplicate
17098	128 [824; D-Sedoheptulose-66	Glycic acid-3-phosphate	45	-0.366	-0.473	10,964	0.391	125	16	116	25	58	93 duplicate
9855	128 [824; D-Sedoheptulose-131	[626; 5-Methylthioadenosine (3TMS)]	38	-0.368	-0.547	18,470	0.500	126	15	127	14	103	62 original
13805	128 [824; D-Sedoheptulose-31	[822; Parabanic acid (2TMS)]	45	-0.374	-0.518	14,752	0.402	127	14	124	17	82	89 duplicate
13359	128 [824; D-Sedoheptulose-27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	34	-0.380	-0.668	22,844	0.342	128	13	136	5	128	115 duplicate
14949	128 [824; D-Sedoheptulose-42	Glutamic acid	41	-0.380	-0.592	21,587	0.253	129	12	129	12	120	133 duplicate
13914	128 [824; D-Sedoheptulose-32	[728; N,N-Dimethyllysine methyl ester]	44	-0.381	-0.620	20,894	0.392	130	11	131	10	115	92 duplicate
10209	128 [824; D-Sedoheptulose-2	Serine	43	-0.408	-0.501	17,675	0.256	131	10	121	20	99	132 duplicate
11285	128 [824; D-Sedoheptulose-10	Glycine	43	-0.408	-0.501	17,675	0.256	131	10	121	20	99	132 duplicate
10484	128 [824; D-Sedoheptulose-4	Phosphoric acid	33	-0.413	-0.750	12,614	0.622	132	9	139	2	67	12 duplicate
16145	128 [824; D-Sedoheptulose-55	[612; 4-Aminobutyric acid (2TBS)]	25	-0.413	-0.419	24,854	0.205	133	8	110	31	132	137 duplicate
16470	128 [824; D-Sedoheptulose-58	[636; 4R-Acetylarnido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	45	-0.414	-0.472	13,644	0.321	135	6	115	26	75	124 duplicate
12540	128 [824; D-Sedoheptulose-20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	15	-0.428	-0.820	14,476	0.335	138	5	140	1	80	120 duplicate
18103	128 [824; D-Sedoheptulose-81	Tyrosine	45	-0.438	-0.623	21,826	0.541	137	4	132	9	122	43 duplicate
17728	128 [824; D-Sedoheptulose-75	Lysine	45	-0.448	-0.543	29,444	0.337	138	3	126	15	137	118 duplicate
10820	128 [824; D-Sedoheptulose-5	Leucine	26	-0.471	-0.588	13,184	0.152	139	2	128	13	73	140 duplicate
16970	128 [824; D-Sedoheptulose-98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	31	-0.553	-0.745	21,298	0.385	140	1	138	3	117	101 duplicate
15336	129 [840; Maltose methoxya	46	59	0.868	0.979	10,486	0.888	1	141	2	140	29	3 duplicate
9870	129 [840; Maltose methoxya	134	59	0.850	0.981	20,448	0.693	2	140	1	141	92	1 original
13015	129 [840; Maltose methoxya	24	59	0.838	0.975	29,729	0.690	3	139	4	138	122	2 duplicate
11673	129 [840; Maltose methoxya	13	59	0.834	0.968	13,140	0.666	4	138	6	136	46	11 duplicate
16388	129 [840; Maltose methoxya	57	54	0.831	0.964	5,055	0.663	5	137	7	135	4	14 duplicate
12051	129 [840; Maltose methoxya	16	59	0.825	0.961	16,298	0.658	6	136	8	134	71	16 duplicate
15706	129 [840; Maltose methoxya	50	58	0.811	0.961	17,257	0.613	7	135	8	133	77	35 duplicate

16304	129 [840; Maltose methoxys	56	[829; Orolic acid (3TMS)]	59	0.811	0.972	3.937	0.673	8	134	5	137	2	8 duplicate
17024	129 [840; Maltose methoxys	65	[646; 3-Deoxyglucitol (5TMS)]	59	0.806	0.977	3.085	0.685	9	133	3	139	1	5 duplicate
18389	129 [840; Maltose methoxys	86	[793; D-Galactono-1,4-lactone (4TMS)]	56	0.786	0.958	15.167	0.686	10	132	10	132	68	4 duplicate
14650	129 [840; Maltose methoxys	39	[829; 1-Phenylethanol (1TMS)]	59	0.771	0.956	10.681	0.632	11	131	11	131	32	27 duplicate
18013	129 [840; Maltose methoxys	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	0.768	0.943	10.175	0.645	12	130	12	130	27	22 duplicate
12175	129 [840; Maltose methoxys	17	[700; 2-methyl-1,2-propanediol (2TMS)]	59	0.762	0.926	16.819	0.590	13	129	16	126	68	45 duplicate
13585	129 [840; Maltose methoxys	29	Erythritol	59	0.759	0.930	9.758	0.585	14	128	14	128	24	49 duplicate
18496	129 [840; Maltose methoxys	88	Gluconic acid	59	0.755	0.920	8.484	0.664	15	127	18	124	14	13 duplicate
16060	129 [840; Maltose methoxys	54	[NA]	52	0.715	0.923	8.945	0.604	16	126	17	125	15	38 duplicate
16793	129 [840; Maltose methoxys	62	[812; D-Xylofuranose (4TMS)]	59	0.702	0.929	14.295	0.631	17	125	15	127	55	28 duplicate
11416	129 [840; Maltose methoxys	11	Succinic acid	59	0.674	0.889	10.144	0.559	18	124	21	121	26	65 duplicate
14548	129 [840; Maltose methoxys	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	59	0.669	0.940	8.996	0.617	19	123	13	129	16	33 duplicate
19171	129 [840; Maltose methoxys	103	[648; Ethylamine (2TMS)]	59	0.649	0.822	9.202	0.548	20	122	31	111	21	68 duplicate
18698	129 [840; Maltose methoxys	92	[680; Glycerol-2-phosphate (4TMS)]	52	0.643	0.789	6.539	0.585	21	121	27	105	7	51 duplicate
19244	129 [840; Maltose methoxys	105	[705; 2-Ketogluconic acid (5TMS)]	48	0.631	0.857	5.940	0.616	22	120	36	116	6	34 duplicate
18928	129 [840; Maltose methoxys	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	0.611	0.817	14.543	0.557	23	119	32	110	58	66 duplicate
11800	129 [840; Maltose methoxys	14	Fumaric acid	59	0.610	0.810	10.681	0.583	24	118	19	123	33	52 duplicate
10071	129 [840; Maltose methoxys	1	[938; Sulfuric acid (2TMS)]	36	0.597	0.720	9.158	0.621	25	117	44	98	20	31 duplicate
11545	129 [840; Maltose methoxys	12	Glyceric acid	58	0.596	0.844	11.915	0.588	26	116	27	115	39	46 duplicate
12780	129 [840; Maltose methoxys	22	[690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.588	0.881	10.628	0.570	27	115	22	120	30	57 duplicate
17794	129 [840; Maltose methoxys	76	Fructose	59	0.565	0.880	22.759	0.648	28	114	24	118	102	20 duplicate
17389	129 [840; Maltose methoxys	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	52	0.560	0.594	18.625	0.509	29	113	58	84	83	82 duplicate
17596	129 [840; Maltose methoxys	73	[708; Glucose methoxyamine (5TMS)]	52	0.557	0.744	7.521	0.519	30	112	41	101	11	78 duplicate
13473	129 [840; Maltose methoxys	28	Malic acid	59	0.550	0.721	9.058	0.491	32	110	43	99	19	90 duplicate
18094	129 [840; Maltose methoxys	101	[832; Dopamine (4TMS)]	59	0.552	0.896	11.043	0.603	31	111	20	122	34	40 duplicate
17921	129 [840; Maltose methoxys	78	Mannose	57	0.527	0.825	7.440	0.573	33	109	33	109	132	56 duplicate
19279	129 [840; Maltose methoxys	106	[733; Threitol (4TMS)]	57	0.521	0.836	7.660	0.568	35	107	29	113	12	62 duplicate
17996	129 [840; Maltose methoxys	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	44	0.507	0.806	4.474	0.658	36	106	34	108	3	18 duplicate
18849	129 [840; Maltose methoxys	91	[768; beta-D-Sedoheptulose-7-phosphate (7TMS)]	59	0.500	0.865	13.045	0.444	37	105	52	90	43	17 duplicate
14238	129 [840; Maltose methoxys	35	Pyroglutamic acid	59	0.494	0.863	39.474	0.643	38	104	25	117	139	23 duplicate
19754	129 [840; Maltose methoxys	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	59	0.492	0.789	28.752	0.604	39	103	36	106	123	38 duplicate
12661	129 [840; Maltose methoxys	21	[678; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	59	0.482	0.717	16.678	0.525	40	102	45	97	73	75 duplicate
19549	129 [840; Maltose methoxys	115	Glucose-6-phosphate	58	0.466	0.843	23.228	0.637	42	100	28	114	104	24 duplicate
19664	129 [840; Maltose methoxys	120	[945; Uridine (3TMS)]	54	0.465	0.338	13.408	0.586	43	99	71	71	49	48 duplicate
13246	129 [840; Maltose methoxys	26	Citramalic acid	59	0.461	0.768	17.247	0.519	44	98	39	103	76	77 duplicate
18443	129 [840; Maltose methoxys	87	[945; beta-D-Glucopyranose (5TMS)]	57	0.429	0.741	32.603	0.585	45	97	42	100	130	50 duplicate
19598	129 [840; Maltose methoxys	117	[724; Glycerol (3TMS)]	55	0.410	0.746	8.007	0.561	46	96	40	102	13	61 duplicate
19409	129 [840; Maltose methoxys	110	[715; Erythritol (4TMS)]	53	0.408	0.787	9.054	0.660	47	95	38	104	18	15 duplicate
18334	129 [840; Maltose methoxys	85	[529; Methylcitric acid (4TMS)]	43	0.404	0.682	9.029	0.408	48	94	50	92	17	124 duplicate
19054	129 [840; Maltose methoxys	100	[857; Mannitol (6TMS)]	59	0.398	0.697	11.446	0.576	49	93	48	94	37	54 duplicate
19694	129 [840; Maltose methoxys	121	[657; Erythritol (4TMS)]	52	0.397	0.702	13.808	0.587	50	92	47	95	52	47 duplicate
19703	129 [840; Maltose methoxys	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	51	0.395	0.803	14.103	0.603	51	91	35	107	53	39 duplicate
19468	129 [840; Maltose methoxys	6	Glycerol	58	0.374	0.602	17.760	0.531	52	90	57	85	78	74 duplicate
10756	129 [840; Maltose methoxys	102	[904; Galactose methoxyamine (5TMS)]	59	0.351	0.666	40.198	0.582	53	89	51	91	140	60 duplicate
19133	129 [840; Maltose methoxys	132	[895; Isomaltose methoxyamine (8TMS)]	59	0.347	0.592	11.074	0.555	54	88	59	83	36	67 duplicate
19868	129 [840; Maltose methoxys	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	41	0.329	0.881	13.676	0.630	55	87	23	119	51	29 original
19783	129 [840; Maltose methoxys	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	39	0.314	0.631	7.218	0.678	56	86	55	87	9	6 duplicate
15145	129 [840; Maltose methoxys	47	[NA]	48	0.287	0.664	6.774	0.656	57	85	53	89	8	19 duplicate
15430	129 [840; Maltose methoxys	47	[NA]	59	0.286	0.311	13.050	0.434	58	84	74	68	44	117 duplicate

135	9871	129 [840; Maltose methoxy	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	59	0.274	0.499	14,630	0.476	59	83	64	78	59	97 original
	19769	129 [840; Maltose methoxy	[559; Erythritol (4TMS)]	45	0.263	0.548	9,914	0.648	80	82	82	80	25	21 duplicate
	17663	129 [840; Maltose methoxy	74 [912; Tetradecanoic acid (1TMS)]	59	0.246	0.554	10,556	0.480	81	81	61	81	31	95 duplicate
	12298	129 [840; Maltose methoxy	18 [590; 1-Acetyl-2-thiohydantoin]	59	0.243	0.460	11,589	0.423	82	80	87	75	38	119 duplicate
	18746	129 [840; Maltose methoxy	93 [607; Putrescine (4TMS)]	56	0.236	0.330	17,228	0.408	63	79	72	70	75	123 duplicate
	19486	129 [840; Maltose methoxy	113 Galactose-6-phosphate	58	0.234	0.708	9,328	0.569	64	78	48	96	22	58 duplicate
	18044	129 [840; Maltose methoxy	80 [772; D-Glucose (5TMS)]	57	0.209	0.618	28,593	0.532	65	76	56	88	121	72 duplicate
	18278	129 [840; Maltose methoxy	84 Mannitol	57	0.209	0.499	29,759	0.468	66	77	63	79	124	102 duplicate
	19208	129 [840; Maltose methoxy	1795; Erythritol (4TMS)]	58	0.203	0.427	11,055	0.559	67	75	68	74	35	84 duplicate
	15973	129 [840; Maltose methoxy	53 Glycerol-2-phosphate	59	0.200	0.175	14,492	0.387	68	74	80	62	56	128 duplicate
	19574	129 [840; Maltose methoxy	116 [882; Pseudouridine (5TMS)]	29	0.192	0.364	9,472	0.451	69	73	70	72	23	109 duplicate
	12420	129 [840; Maltose methoxy	19 Alanine (BP) (3TMS)	59	0.190	0.587	12,651	0.581	70	72	60	82	41	53 duplicate
	14851	129 [840; Maltose methoxy	41 [639; Proline (2TMS)]	59	0.156	0.465	14,722	0.523	71	71	66	76	60	76 duplicate
	19523	129 [840; Maltose methoxy	114 Fructose-6-phosphate	51	0.153	0.685	10,255	0.620	72	70	49	93	28	32 duplicate
	18884	129 [840; Maltose methoxy	96 myo-Inositol	44	0.144	0.196	18,600	0.368	73	69	79	63	82	136 duplicate
	19721	129 [840; Maltose methoxy	123 [945; Galactofuranose-6-phosphate (7TMS)]	59	0.107	0.410	13,355	0.564	74	68	69	73	48	59 duplicate
	18599	129 [840; Maltose methoxy	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	59	0.080	0.059	12,719	0.441	75	67	84	58	42	113 duplicate
	9876	129 [840; Maltose methoxy	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	44	0.072	0.253	16,272	0.483	76	66	75	67	70	94 original
	9869	129 [840; Maltose methoxy	133 [855; Squalene]	59	0.059	0.053	13,308	0.377	77	65	85	57	47	134 original
	16871	129 [840; Maltose methoxy	63 Glutamine	47	0.047	-0.683	23,599	0.673	78	64	116	26	106	9 duplicate
	18221	129 [840; Maltose methoxy	83 Sorbitol	53	0.044	-0.349	24,171	0.321	79	63	95	47	110	139 duplicate
	19439	129 [840; Maltose methoxy	111 [583; Erythritol (4TMS)]	40	0.018	0.161	21,768	0.470	80	82	81	61	97	101 duplicate
	19378	129 [840; Maltose methoxy	109 Octadecanoic acid	59	0.006	0.315	21,940	0.475	81	61	73	69	99	98 duplicate
	16948	129 [840; Maltose methoxy	64 [789; Tyramine (3TMS)]	59	-0.004	0.138	12,127	0.461	82	60	83	59	40	104 duplicate
	17528	129 [840; Maltose methoxy	72 [919; D-Xylopyranose (4TMS)]	58	-0.008	-0.055	14,522	0.346	83	59	89	53	57	138 duplicate
	17983	129 [840; Maltose methoxy	79 Glucose	59	-0.010	0.478	33,904	0.592	84	58	65	77	133	44 duplicate
	9877	129 [840; Maltose methoxy	141 Lanosta-8,24-dien-3-beta-ol	56	-0.019	0.140	15,926	0.519	85	57	82	60	69	78 original
	9875	129 [840; Maltose methoxy	139 [700; Ergosta-5,7-dien-3-ol]	34	-0.020	0.039	19,367	0.506	86	56	87	55	85	83 original
	11826	129 [840; Maltose methoxy	15 Alanine	59	-0.020	0.017	19,715	0.664	87	55	77	65	86	12 duplicate
	19643	129 [840; Maltose methoxy	119 [931; myo-Inositol-2-phosphate (7TMS)]	59	-0.026	-0.016	13,531	0.501	88	54	88	54	50	84 duplicate
	18621	129 [840; Maltose methoxy	118 [928; Glucopyranose-6-phosphate (6TMS)]	57	-0.034	0.211	13,137	0.445	89	53	78	64	45	111 duplicate
	15885	129 [840; Maltose methoxy	52 [NA]	41	-0.034	-0.553	24,418	0.633	90	52	104	38	112	25 duplicate
	18793	129 [840; Maltose methoxy	94 Hexadecanoic acid	59	-0.051	0.249	21,611	0.496	91	51	76	88	95	87 duplicate
	19313	129 [840; Maltose methoxy	107 9-(Z)-Octadecenoic acid	59	-0.056	-0.167	16,901	0.427	92	50	91	51	74	118 duplicate
	9872	129 [840; Maltose methoxy	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.118	-0.354	5,567	0.512	93	49	96	46	5	81 original
	9873	129 [840; Maltose methoxy	137 Ergosterol	59	-0.121	-0.133	17,855	0.459	94	48	90	52	80	106 original
	9874	129 [840; Maltose methoxy	138 [674; Ergosterol (1TMS)]	42	-0.166	0.040	18,241	0.462	95	47	86	56	81	103 original
		129 [840; Maltose methoxy	[734; 1-Monoleoylglycerol (2TMS); 1-Monohexadecenylglycerol (1TMS)]	54	-0.168	-0.244	24,755	0.410	96	46	92	50	116	122 duplicate
	19738	129 [840; Maltose methoxy	43 [548; Leucine (2TBS)]	55	-0.205	-0.411	14,960	0.455	97	45	97	45	63	108 duplicate
	10485	129 [840; Maltose methoxy	4 Phosphoric acid	46	-0.223	-0.417	34,463	0.265	98	44	98	44	136	141 duplicate
	9866	129 [840; Maltose methoxy	130 Trehalose	59	-0.229	-0.280	29,846	0.386	99	43	93	49	125	130 original
	17459	129 [840; Maltose methoxy	71 [731; Erythrose (3TMS)]	59	-0.261	-0.311	15,707	0.416	100	42	94	48	67	120 duplicate
	19346	129 [840; Maltose methoxy	108 Octadecenoic acid	59	-0.276	-0.431	14,885	0.405	101	41	99	43	61	125 duplicate
	16714	129 [840; Maltose methoxy	61 [NA]	59	-0.279	-0.485	14,207	0.518	102	40	101	41	54	80 duplicate
	13131	129 [840; Maltose methoxy	25 [709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.303	-0.870	23,000	0.623	103	39	135	7	103	30 duplicate
		129 [840; Maltose methoxy	[636; 4R-Acetimido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	58	-0.334	-0.431	20,225	0.355	104	38	100	42	91	137 duplicate
	16471	129 [840; Maltose methoxy	68 [570; Hypoxanthine (2TMS)]	17	-0.338	-0.900	15,144	0.499	105	37	137	5	65	85 duplicate
	18971	129 [840; Maltose methoxy	98 [697; Ribose-5-phosphate methoxamine (5TMS)]	44	-0.345	-0.771	22,479	0.497	106	36	123	19	100	88 duplicate



18548	129 [840; Maltose methoxys	89	[775; Dopamine (4TMS)]	30	-0.370	-0.805	21,785	0.539	107	35	126	16	98	70 duplicate
12898	129 [840; Maltose methoxys	23	Homoserine	59	-0.371	-0.805	20,166	0.543	108	34	127	15	90	69 duplicate
17729	129 [840; Maltose methoxys	75	Lysine	59	-0.373	-0.538	38,181	0.405	109	32	102	40	138	126 duplicate
15615	129 [840; Maltose methoxys	49	[877; Pyrophosphoric acid (4TMS)]	59	-0.373	-0.538	25,200	0.478	110	33	103	39	118	96 duplicate
13360	129 [840; Maltose methoxys	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	48	-0.379	-0.776	24,546	0.460	111	31	124	18	114	105 duplicate
9867	129 [840; Maltose methoxys	131	[626; 5-Methylthiadenosine (3TMS)]	50	-0.417	-0.652	19,771	0.593	112	30	113	29	87	43 original
14341	129 [840; Maltose methoxys	38	[596; N-Acetylglutamic acid (2TMS)]	59	-0.430	-0.593	29,988	0.397	113	28	107	35	126	128 duplicate
15241	129 [840; Maltose methoxys	45	Homocysteine	58	-0.447	-0.633	23,885	0.434	114	28	108	34	107	116 duplicate
18839	129 [840; Maltose methoxys	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	45	-0.461	-0.639	21,633	0.472	115	27	111	31	96	99 duplicate
10890	129 [840; Maltose methoxys	48	Asparagine	59	-0.465	-0.583	30,563	0.370	116	26	106	36	127	135 duplicate
15523	129 [840; Maltose methoxys	7	Threonine	59	-0.483	-0.848	21,154	0.669	117	25	133	9	93	10 duplicate
17173	129 [840; Maltose methoxys	67	Citric acid	59	-0.483	-0.636	24,691	0.410	118	24	109	33	115	121 duplicate
10210	129 [840; Maltose methoxys	2	Serine	57	-0.506	-0.639	25,506	0.385	119	23	110	32	119	132 duplicate
14130	129 [840; Maltose methoxys	34	Aspartic acid	59	-0.520	-0.645	33,924	0.440	120	21	112	30	134	114 duplicate
13806	129 [840; Maltose methoxys	31	[622; Parabenic acid (2TMS)]	59	-0.520	-0.729	17,769	0.488	121	22	121	21	79	92 duplicate
17099	129 [840; Maltose methoxys	68	Glyceric acid-3-phosphate	59	-0.545	-0.696	14,942	0.491	122	20	117	25	82	91 duplicate
11023	129 [840; Maltose methoxys	8	Isoleucine	50	-0.546	-0.568	24,503	0.280	123	19	105	37	113	140 duplicate
16634	129 [840; Maltose methoxys	60	Glycerol-3-phosphate	59	-0.546	-0.652	23,530	0.532	124	18	114	28	105	73 duplicate
14445	129 [840; Maltose methoxys	37	Phenylalanine	59	-0.565	-0.732	24,315	0.493	125	17	122	20	111	89 duplicate
14023	129 [840; Maltose methoxys	33	Methionine	59	-0.568	-0.699	19,777	0.451	126	16	118	24	88	110 duplicate
11155	129 [840; Maltose methoxys	9	Proline	58	-0.575	-0.679	32,174	0.386	127	15	115	27	128	131 duplicate
15796	129 [840; Maltose methoxys	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	39	-0.590	-0.827	20,024	0.493	128	14	130	12	89	88 duplicate
13698	129 [840; Maltose methoxys	30	[815; Ethyl-3(2H)-thiophenone]	59	-0.627	-0.710	32,321	0.396	129	13	119	23	129	127 duplicate
13915	129 [840; Maltose methoxys	32	[729; N,N-Dimethyllysine methyl ester]	58	-0.631	-0.840	24,980	0.538	130	12	132	10	117	71 duplicate
12541	129 [840; Maltose methoxys	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	26	-0.637	-0.910	14,961	0.604	131	11	139	3	64	37 duplicate
16146	129 [840; Maltose methoxys	55	[612; 4-Aminobutyric acid (2TBS)]	38	-0.639	-0.833	21,384	0.560	132	10	131	11	94	63 duplicate
15553	129 [840; Maltose methoxys	59	Ornithine; Arginine	59	-0.641	-0.726	40,536	0.458	133	9	120	22	141	107 duplicate
10348	129 [840; Maltose methoxys	3	Ethanolamine	57	-0.650	-0.858	18,092	0.595	134	8	134	8	84	42 duplicate
17318	129 [840; Maltose methoxys	69	Arginine	55	-0.658	-0.896	26,786	0.575	135	7	136	6	120	55 duplicate
11286	129 [840; Maltose methoxys	10	Glycine	59	-0.667	-0.948	23,929	0.673	136	6	141	1	108	7 duplicate
17858	129 [840; Maltose methoxys	77	[826; beta-[(5-methyl-2-thienyl)methyl]eneamino-benzeneacetic acid methyl ester]	57	-0.682	-0.819	33,044	0.485	137	5	129	13	131	93 duplicate
18163	129 [840; Maltose methoxys	82	Lysine	34	-0.690	-0.945	22,753	0.602	138	4	140	2	101	41 duplicate
10621	129 [840; Maltose methoxys	5	Leucine	40	-0.715	-0.792	16,423	0.382	139	3	125	17	72	133 duplicate
14950	129 [840; Maltose methoxys	42	Glutamic acid	55	-0.732	-0.805	33,962	0.437	140	2	128	14	135	115 duplicate
18104	129 [840; Maltose methoxys	81	Tyrosine	59	-0.732	-0.902	35,781	0.633	141	1	138	4	137	28 duplicate
17730	130 Trehalose	75	Lysine	63	0.467	0.578	10,444	0.406	1	141	1	141	13	37 duplicate
16472	130 Trehalose	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	63	0.464	0.544	17,181	0.384	2	140	2	140	38	70 duplicate
14342	130 Trehalose	36	[596; N-Acetylglutamic acid (2TMS)]	63	0.359	0.538	6,192	0.431	3	139	3	139	3	13 duplicate
17100	130 Trehalose	66	Glyceric acid-3-phosphate	63	0.327	0.502	30,615	0.410	4	138	4	138	97	33 duplicate
10211	130 Trehalose	2	Serine	61	0.281	0.456	20,869	0.389	5	137	7	135	50	60 duplicate
17994	130 Trehalose	79	Glucose	63	0.264	0.106	9,478	0.428	6	136	49	83	8	18 duplicate
18972	130 Trehalose	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	47	0.258	0.470	40,099	0.359	7	135	6	136	129	107 duplicate
11156	130 Trehalose	9	Proline	62	0.249	0.475	16,358	0.376	8	134	5	137	35	84 duplicate
13916	130 Trehalose	32	[728; N,N-Dimethyllysine methyl ester]	62	0.243	0.408	36,805	0.371	9	133	10	132	120	90 duplicate
12542	130 Trehalose	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	30	0.241	0.225	31,419	0.340	10	132	36	106	102	122 duplicate
13807	130 Trehalose	31	[622; Parabenic acid (2TMS)]	63	0.230	0.350	35,257	0.378	11	131	14	128	116	79 duplicate
10349	130 Trehalose	3	Ethanolamine	61	0.230	0.294	34,924	0.390	12	130	23	119	115	59 duplicate

19209	130 Trehalose	104 [795; Erythritol (4TMS)]	62	0.224	0.277	28,025	0.403	13	129	27	115	82	39 duplicate
14951	130 Trehalose	42 Glutamic acid	59	0.223	0.363	15,685	0.333	14	128	12	130	33	132 duplicate
18105	130 Trehalose	81 Tyrosine	63	0.222	0.344	10,357	0.428	15	127	15	127	12	17 duplicate
19739	130 Trehalose	[734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]	58	0.221	0.420	49,008	0.388	16	126	9	133	140	64 duplicate
16554	130 Trehalose	59 Ornithine; Arginine	63	0.219	0.396	11,883	0.339	17	125	11	131	16	125 duplicate
11287	130 Trehalose	10 Glycine	63	0.215	0.314	15,054	0.400	18	124	19	123	30	44 duplicate
10891	130 Trehalose	7 Threonine	63	0.198	0.446	3,334	0.391	19	123	8	134	1	56 duplicate
9885	130 Trehalose	138 [674; Ergosterol (1TMS)]	45	0.198	0.264	36,892	0.394	20	122	29	113	121	53 original
9885	130 Trehalose	23 Homoserine	63	0.188	0.360	27,180	0.368	21	121	13	129	76	94 duplicate
13361	130 Trehalose	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	52	0.175	0.303	38,759	0.395	22	120	22	120	127	48 duplicate
16949	130 Trehalose	64 [789; Tyramine (3TMS)]	63	0.175	0.140	28,235	0.368	23	119	45	97	90	98 duplicate
9880	130 Trehalose	133 [855; Squalene]	63	0.174	0.307	27,413	0.382	24	118	21	121	77	73 original
19722	130 Trehalose	123 [945; Galactofuranose-6-phosphate (7TMS)]	63	0.172	0.238	21,118	0.419	25	117	32	110	51	24 duplicate
17859	130 Trehalose	[826; beta-[[5-methyl-2-phenyl]methyl]pentamino-benzeneacetic acid methyl ester]	61	0.160	0.327	12,911	0.339	26	116	16	128	19	128 duplicate
9878	130 Trehalose	131 [626; 5-Methylthioadenosine (3TMS)]	54	0.152	0.246	39,773	0.290	27	115	30	112	128	140 original
10488	130 Trehalose	4 Phosphoric acid	50	0.151	0.226	7,003	0.360	28	114	35	107	4	108 duplicate
11927	130 Trehalose	15 Alanine	63	0.148	0.135	14,793	0.377	29	113	46	96	29	80 duplicate
13697	130 Trehalose	30 [815; Ethyl-3-(2H)-thiophenone]	63	0.137	0.293	10,684	0.364	30	112	24	118	14	99 duplicate
15974	130 Trehalose	53 Glycerol-2-phosphate	63	0.132	0.229	36,124	0.344	31	111	34	108	117	118 duplicate
16635	130 Trehalose	60 Glycerol-3-phosphate	63	0.126	0.235	10,214	0.417	32	110	33	109	11	25 duplicate
15797	130 Trehalose	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	43	0.123	0.307	40,271	0.313	33	109	20	122	131	137 duplicate
19347	130 Trehalose	108 Octadecenoic acid	63	0.122	0.324	31,244	0.358	34	108	17	125	99	109 duplicate
17174	130 Trehalose	67 Citric acid	63	0.118	0.286	7,161	0.378	35	107	28	116	5	78 duplicate
14131	130 Trehalose	34 Aspartic acid	63	0.112	0.184	8,023	0.342	36	106	41	101	6	121 duplicate
12421	130 Trehalose	19 Alanine (BP) (3TMS)	63	0.110	0.055	21,324	0.369	37	105	57	85	52	92 duplicate
14024	130 Trehalose	33 Methionine	63	0.108	0.189	27,561	0.343	38	104	40	102	79	120 duplicate
18794	130 Trehalose	94 Hexadecanoic acid	63	0.100	0.110	13,284	0.362	39	103	48	94	22	103 duplicate
13132	130 Trehalose	25 [709; 2,5-Diaminovalerolactam (2TMS)]	48	0.099	0.316	32,170	0.404	40	102	18	124	106	38 duplicate
14446	130 Trehalose	37 Phenylalanine	63	0.099	0.269	8,383	0.379	41	101	28	114	7	76 duplicate
15524	130 Trehalose	48 Asparagine	63	0.095	0.146	28,486	0.334	42	100	44	88	85	130 duplicate
19524	130 Trehalose	114 Fructose-6-phosphate	53	0.093	0.001	30,336	0.409	43	99	65	77	83	34 duplicate
19379	130 Trehalose	109 Octadecanoic acid	63	0.086	0.085	17,295	0.327	44	98	51	91	39	134 duplicate
18222	130 Trehalose	83 Sorbitol	57	0.069	0.240	12,579	0.380	45	97	31	111	18	75 duplicate
11024	130 Trehalose	8 Isolaucine	54	0.068	0.280	18,861	0.364	46	96	25	117	45	101 duplicate
17319	130 Trehalose	69 Arginine	59	0.063	0.222	15,870	0.391	47	95	37	105	34	58 duplicate
14852	130 Trehalose	41 [839; Proline (2TMS)]	63	0.060	0.064	18,593	0.357	48	94	55	87	44	111 duplicate
15049	130 Trehalose	43 [548; Leucine (2TBS)]	59	0.053	0.056	25,189	0.336	49	93	56	86	66	129 duplicate
19497	130 Trehalose	113 Galactose-6-phosphate	61	0.049	-0.084	31,576	0.462	50	92	80	62	104	8 duplicate
19622	130 Trehalose	118 [928; Glucopyranose-6-phosphate (6TMS)]	58	0.048	0.075	30,590	0.364	51	91	52	90	96	102 duplicate
17460	130 Trehalose	71 [731; Erythrose (3TMS)]	63	0.038	0.179	19,187	0.457	52	90	42	100	48	7 duplicate
9884	130 Trehalose	137 Ergosterol	63	0.037	0.204	21,343	0.336	53	89	39	103	53	128 original
19314	130 Trehalose	107 9-[Z]-Octadecenoic acid	63	0.028	0.213	16,986	0.377	54	88	38	104	37	81 duplicate
17597	130 Trehalose	73 [708; Glucose methoxyamine (5TMS)]	56	0.022	-0.056	31,393	0.344	55	87	73	69	101	119 duplicate
16715	130 Trehalose	61 [NA]	63	0.012	-0.094	27,874	0.351	56	86	81	61	81	112 duplicate
17529	130 Trehalose	72 [919; D-Xylopyranose (4TMS)]	62	0.010	0.039	31,951	0.371	57	85	60	82	105	89 duplicate
15242	130 Trehalose	45 Homocysteine	60	0.000	-0.048	46,502	0.368	58	84	70	72	139	83 duplicate
10757	130 Trehalose	6 Glycerol	63	-0.005	-0.102	12,984	0.361	59	83	82	60	21	105 duplicate
18549	130 Trehalose	89 [775; Dopamine (4TMS)]	34	-0.005	0.167	30,453	0.346	60	82	43	99	85	117 duplicate
19280	130 Trehalose	106 [733; Threitol (4TMS)]	61	-0.011	-0.061	26,175	0.459	61	81	74	68	72	8 duplicate

18045	130	Trehalose	80	[772; D-Glucose (5TMS)]	61	-0.014	-0.001	12.404	0.329	62	80	66	76	17	133 duplicate
9887	130	Trehalose	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	48	-0.021	-0.043	37.968	0.370	63	79	69	73	124	91 original
18840	130	Trehalose	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	49	-0.022	0.029	41.678	0.288	64	78	61	81	133	141 duplicate
9888	130	Trehalose	141	Lanosta-8,24-dien-3-beta-ol	60	-0.024	0.003	38.661	0.382	65	77	64	78	125	104 original
15616	130	Trehalose	49	[877; Pyrophosphoric acid (4TMS)]	63	-0.026	-0.064	44.375	0.359	66	76	75	67	138	108 duplicate
18335	130	Trehalose	85	[528; Methylcitrinic acid (4TMS)]	47	-0.027	-0.078	25.362	0.407	67	75	79	63	68	38 duplicate
18600	130	Trehalose	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	63	-0.031	0.070	26.186	0.348	68	74	53	89	73	113 duplicate
18164	130	Trehalose	82	Lysine	38	-0.033	0.010	17.476	0.411	69	73	63	79	40	30 duplicate
14752	130	Trehalose	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	63	-0.033	-0.105	5.829	0.410	70	72	84	58	2	32 duplicate
19704	130	Trehalose	122	[644; Erythritol (4TMS)]	52	-0.036	-0.142	37.130	0.497	71	71	90	52	122	3 duplicate
19770	130	Trehalose	126	[559; Erythritol (4TMS)]	45	-0.036	-0.049	26.859	0.473	72	70	71	71	75	4 duplicate
19685	130	Trehalose	121	[657; Erythritol (4TMS)]	54	-0.038	-0.040	36.617	0.398	73	69	68	74	119	47 duplicate
10622	130	Trehalose	5	Leucine	44	-0.040	0.067	29.046	0.385	74	68	54	88	89	67 duplicate
17664	130	Trehalose	74	[912; Tetradecanoic acid (1TMS)]	63	-0.040	-0.075	31.540	0.368	75	67	77	65	103	97 duplicate
9886	130	Trehalose	139	[700; Ergosta-6,7-dien-3-ol]	37	-0.042	0.053	37.142	0.421	76	66	58	84	123	22 original
18444	130	Trehalose	87	[945; beta-D-Glucopyranose (5TMS)]	61	-0.050	-0.052	13.640	0.388	77	65	72	70	23	65 duplicate
12289	130	Trehalose	18	[590; 1-Acetyl-2-thiohydantoin]	63	-0.051	-0.105	24.993	0.393	78	64	83	59	65	55 duplicate
19440	130	Trehalose	111	[583; Erythritol (4TMS)]	42	-0.052	0.018	40.203	0.324	79	63	62	80	130	136 duplicate
18575	130	Trehalose	116	[882; Pseudouridine (5TMS)]	30	-0.053	-0.071	23.634	0.427	80	62	76	66	62	19 duplicate
17795	130	Trehalose	76	Fructose	63	-0.061	-0.147	13.760	0.367	81	61	92	50	26	95 duplicate
19410	130	Trehalose	110	[715; Erythritol (4TMS)]	53	-0.071	-0.108	31.292	0.507	82	80	85	57	100	1 duplicate
15146	130	Trehalose	44	[910; 2-Ketogluconic acid methoxymine (4TMS)]	49	-0.071	-0.075	23.467	0.451	83	59	78	64	60	9 duplicate
19755	130	Trehalose	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	63	-0.073	-0.114	11.821	0.338	84	58	88	56	15	127 duplicate
17922	130	Trehalose	78	Mannose	61	-0.081	-0.152	33.192	0.347	85	67	95	47	108	114 duplicate
16872	130	Trehalose	63	Glutamine	51	-0.082	0.101	32.550	0.365	86	56	50	92	107	98 duplicate
9883	130	Trehalose	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.088	0.110	13.756	0.307	87	55	47	95	25	138 original
15886	130	Trehalose	52	[NA]	45	-0.089	0.051	38.682	0.442	88	54	59	83	126	11 duplicate
14237	130	Trehalose	35	Pyroglutamic acid	63	-0.099	-0.190	12.916	0.327	89	53	99	43	20	135 duplicate
19599	130	Trehalose	117	[724; Glyceral (3TMS)]	55	-0.106	-0.148	28.787	0.462	90	52	93	49	87	5 duplicate
18665	130	Trehalose	120	[945; Uridine (3TMS)]	54	-0.110	-0.131	17.939	0.395	91	61	88	54	43	50 duplicate
19644	130	Trehalose	119	[931; myo-Inositol-2-phosphate (7TMS)]	63	-0.113	-0.117	26.837	0.372	92	50	87	55	74	87 duplicate
12662	130	Trehalose	21	[678; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	63	-0.116	-0.211	15.258	0.389	93	49	100	42	31	61 duplicate
18885	130	Trehalose	96	myo-Inositol	63	-0.118	-0.211	15.258	0.378	94	48	89	63	134	110 duplicate
13247	130	Trehalose	26	Citramalic acid	48	-0.121	-0.136	41.746	0.357	94	48	102	40	28	83 duplicate
17390	130	Trehalose	132	[895; 2-Furan-2-hydroxyacetic acid (2TMS)]	63	-0.123	-0.232	14.697	0.376	95	47	102	40	28	83 duplicate
9879	130	Trehalose	115	Glucose-6-phosphate	56	-0.130	-0.024	13.844	0.347	96	46	67	75	27	115 duplicate
19550	130	Trehalose	28	Malic acid	42	-0.134	-0.330	33.775	0.411	97	45	112	30	111	31 original
13474	130	Trehalose	61	myo-Inositol	63	-0.136	-0.184	9.802	0.394	98	44	97	45	10	52 duplicate
18390	130	Trehalose	86	[793; D-Galactono-1,4-lactone (4TMS)]	60	-0.154	-0.223	25.372	0.429	100	42	101	41	69	71 duplicate
19014	130	Trehalose	99	[662; Ribose-5-phosphate methoxymine (BP) (5TMS)]	41	-0.156	-0.145	28.601	0.439	101	41	91	51	88	12 duplicate
15431	130	Trehalose	63	-0.168	63	-0.168	-0.182	29.380	0.420	102	40	96	46	91	23 duplicate
11801	130	Trehalose	14	Fumaric acid	63	-0.173	-0.315	34.245	0.374	103	39	111	31	112	85 duplicate
16147	130	Trehalose	55	[612; 4-Aminobutyric acid (2TBS)]	42	-0.185	-0.149	42.771	0.304	104	38	94	48	136	139 duplicate
15707	130	Trehalose	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	-0.185	-0.282	44.011	0.364	105	37	106	36	137	100 duplicate
12781	130	Trehalose	62	[690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	52	-0.193	-0.340	34.761	0.424	106	36	115	27	114	20 duplicate
16794	130	Trehalose	82	[812; D-Xylofuranose (4TMS)]	63	-0.216	-0.268	17.603	0.394	108	34	103	39	42	51 duplicate
17247	130	Trehalose	68	[570; Hypoxanthine (2TMS)]	19	-0.216	-0.185	27.791	0.340	109	33	98	44	80	124 duplicate
19784	130	Trehalose	127	[777; Fructose-6-phosphate methoxymine (6TMS)]	39	-0.217	-0.360	21.834	0.428	110	32	118	24	55	15 duplicate
14651	130	Trehalose	39	[826; 1-Phenylethanol (1TMS)]	62	-0.219	-0.363	23.003	0.402	111	31	120	22	57	43 duplicate
14549	130	Trehalose	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	63	-0.227	-0.413	25.561	0.391	112	30	129	13	70	57 duplicate

19809	130 Trehalose	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	-0.229	-0.280	29.846	0.388	113	29	105	37	92	66 duplicate
19469	130 Trehalose	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	62	-0.245	-0.369	42.056	0.412	114	28	121	21	135	28 duplicate
11674	130 Trehalose	13 Urcil	63	-0.246	-0.362	48.979	0.403	115	27	119	23	46	40 duplicate
9881	130 Trehalose	134 Isomaltose	63	-0.251	-0.331	17.555	0.398	116	26	113	29	41	46 original
18497	130 Trehalose	88 Gluconic acid	63	-0.252	-0.373	24.324	0.393	117	25	122	20	63	54 duplicate
18134	130 Trehalose	102 [904; Galactose methoxyamine (5TMS)]	63	-0.254	-0.347	30.949	0.399	118	24	117	25	98	45 duplicate
11417	130 Trehalose	11 Succinic acid	63	-0.259	-0.390	24.855	0.377	119	23	126	16	64	82 duplicate
18055	130 Trehalose	100 [857; Mannitol (6TMS)]	63	-0.260	-0.422	23.620	0.423	120	22	130	12	61	21 duplicate
17025	130 Trehalose	65 [646; 3-Deoxyglucitol (5TMS)]	62	-0.261	-0.301	33.644	0.385	121	21	109	33	110	69 duplicate
16305	130 Trehalose	56 [829; Orotic acid (3TMS)]	63	-0.262	-0.341	33.451	0.374	122	20	116	26	109	86 duplicate
13016	130 Trehalose	24 [725; 2-Ketotartaric acid (2TMS)]	63	-0.263	-0.381	9.600	0.381	123	19	124	18	9	74 duplicate
18650	130 Trehalose	91 [766; beta-D-Methylglucopyranoside (4TMS)]	63	-0.267	-0.476	30.423	0.403	124	18	135	7	84	41 duplicate
13588	130 Trehalose	29 Erythritol	63	-0.269	-0.423	28.901	0.382	125	17	131	11	88	72 duplicate
19095	130 Trehalose	101 [832; Dopamine (4TMS)]	63	-0.271	-0.485	28.029	0.372	126	16	137	5	83	88 duplicate
12052	130 Trehalose	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	63	-0.273	-0.408	15.506	0.385	127	14	128	14	32	63 duplicate
12176	130 Trehalose	17 [700; 2-methyl-1,2-propanediol (2TMS)]	63	-0.273	-0.456	16.904	0.388	128	15	133	9	38	63 duplicate
15337	130 Trehalose	46 Arabinose	63	-0.283	-0.337	25.324	0.379	129	13	114	28	67	77 duplicate
19172	130 Trehalose	103 [646; Ethylamine (2TMS)]	62	-0.285	-0.470	27.431	0.415	130	12	134	8	78	28 duplicate
16389	130 Trehalose	57 [757; 2-Desoxy-pentose-3-ylose dimethoxyamine (2TMS)]	55	-0.309	-0.276	25.969	0.416	131	11	104	38	71	27 duplicate
10072	130 Trehalose	1 [938; Sulfuric acid (2TMS)]	36	-0.317	-0.403	23.326	0.449	132	10	127	15	58	10 duplicate
19797	130 Trehalose	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45	-0.321	-0.515	21.622	0.416	133	9	138	4	54	26 duplicate
18929	130 Trehalose	97 [756; beta-D-Methylglucopyranoside (4TMS)]	52	-0.323	-0.373	20.145	0.395	134	8	123	19	49	49 duplicate
9882	130 Trehalose	135	63	-0.323	-0.382	19.067	0.430	135	7	125	17	47	14 original
11546	130 Trehalose	12 Glycetic acid	62	-0.339	-0.481	36.228	0.408	136	6	136	6	118	35 duplicate
16061	130 Trehalose	54 [NA]	55	-0.371	-0.446	34.755	0.340	137	5	132	10	113	123 duplicate
18747	130 Trehalose	83 [607; Putrescine (4TMS)]	59	-0.383	-0.523	40.576	0.389	138	4	139	3	132	62 duplicate
18279	130 Trehalose	84 Mannitol	61	-0.393	-0.575	13.735	0.500	139	3	140	2	24	2 duplicate
18699	130 Trehalose	92 [680; Glycerol-2-phosphate (4TMS)]	54	-0.398	-0.299	28.166	0.333	140	2	108	34	84	131 duplicate
19245	130 Trehalose	105 [705; 2-Ketogluconic acid (5TMS)]	48	-0.473	-0.628	23.374	0.403	141	1	141	1	59	42 duplicate
12543	131 [626; 5-Methylthioadenosine]	20 [619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	27	0.738	0.914	5.417	0.885	1	141	2	140	1	1 duplicate
15525	131 [626; 5-Methylthioadenosine]	48 Asparagine	55	0.636	0.797	16.508	0.598	2	140	5	137	58	17 duplicate
13133	131 [626; 5-Methylthioadenosine]	25 [709; 2,5-Diaminovalerolactam (2TMS)]	41	0.622	0.622	13.198	0.519	3	139	16	126	40	57 duplicate
18165	131 [626; 5-Methylthioadenosine]	82 Lysine	34	0.615	0.856	21.615	0.638	4	138	3	139	82	2 duplicate
11288	131 [626; 5-Methylthioadenosine]	10 Glycine	55	0.596	0.745	28.287	0.630	5	137	8	134	105	4 duplicate
14952	131 [626; 5-Methylthioadenosine]	42 Glutamic acid	51	0.591	0.408	37.694	0.434	6	136	29	113	122	110 duplicate
15798	131 [626; 5-Methylthioadenosine]	51 [489; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	38	0.582	0.689	6.626	0.524	7	135	13	129	5	52 duplicate
15617	131 [626; 5-Methylthioadenosine]	49 [877; Pyrophosphoric acid (4TMS)]	55	0.580	0.760	7.316	0.493	8	134	7	135	11	80 duplicate
17248	131 [626; 5-Methylthioadenosine]	68 [570; Hypoxanthine (2TMS)]	15	0.562	0.931	5.462	0.554	9	133	1	141	2	40 duplicate
10623	131 [626; 5-Methylthioadenosine]	5 Leucine	40	0.546	0.656	10.082	0.495	10	132	14	128	25	79 duplicate
16148	131 [626; 5-Methylthioadenosine]	55 [612; 4-Aminobutyric acid (2TMS)]	38	0.533	0.720	8.775	0.608	11	131	10	132	18	11 duplicate
16873	131 [626; 5-Methylthioadenosine]	63 Glutamine	43	0.515	0.718	12.950	0.513	12	130	11	131	37	64 duplicate
17320	131 [626; 5-Methylthioadenosine]	69 Arginine	21	0.507	0.573	30.017	0.562	13	129	17	125	109	36 duplicate
18550	131 [626; 5-Methylthioadenosine]	89 [775; Dopamine (4TMS)]	28	0.497	0.850	9.398	0.622	14	128	4	138	23	7 duplicate
18106	131 [626; 5-Methylthioadenosine]	3 Tyrosine	55	0.492	0.509	42.982	0.616	15	127	20	122	134	9 duplicate
10350	131 [626; 5-Methylthioadenosine]	8 Ethanolamine	54	0.468	0.570	9.124	0.603	16	126	18	124	20	16 duplicate
15887	131 [626; 5-Methylthioadenosine]	52 [NA]	40	0.464	0.768	8.746	0.607	17	125	6	136	15	12 duplicate
16716	131 [626; 5-Methylthioadenosine]	61 [NA]	55	0.445	0.496	14.734	0.484	18	124	22	120	51	85 duplicate

17860	131 [626; 5-Methylthioadeno	[826; beta-[[[5-methyl-2-thienyl]methyl]eneamino-	54	0.444	0.409	38.654	0.451	19	123	28	114	124	99 duplicate
18841	131 [626; 5-Methylthioadeno	benzeneacetic acid methyl ester]	44	0.442	0.710	6.575	0.589	20	122	12	130	4	23 duplicate
13698	131 [626; 5-Methylthioadeno	[770; 3,4,6-Trisubstituted phenylthioaniline (5TMS)]	55	0.436	0.373	39.006	0.391	21	121	31	111	125	128 duplicate
16555	131 [626; 5-Methylthioadeno	[815; Ethyl-3-(2H)-thiophenone]	55	0.434	0.375	49.984	0.396	22	120	30	112	139	128 duplicate
19348	131 [626; 5-Methylthioadeno	Omitiline; Arginine	55	0.428	0.417	12.078	0.393	23	119	27	115	33	127 duplicate
18973	131 [626; 5-Methylthioadeno	Octadecanoic acid	45	0.416	0.729	6.217	0.478	24	118	9	133	3	87 duplicate
14025	131 [626; 5-Methylthioadeno	[697; Ribose-5-phosphate methoxyamine (5TMS)]	55	0.383	0.370	17.684	0.438	25	117	32	110	68	108 duplicate
13917	131 [626; 5-Methylthioadeno	Methionine	54	0.367	0.424	13.694	0.552	26	116	26	116	44	41 duplicate
12900	131 [626; 5-Methylthioadeno	[729; N,N-Dimethyllysine methyl ester]	55	0.366	0.654	17.474	0.502	27	115	15	127	67	73 duplicate
15243	131 [626; 5-Methylthioadeno	Homocysteine	53	0.364	0.485	6.683	0.413	28	114	24	118	7	118 duplicate
14132	131 [626; 5-Methylthioadeno	Aspartic acid	55	0.360	0.358	42.258	0.404	29	113	34	108	132	123 duplicate
13808	131 [626; 5-Methylthioadeno	[622; Parabanic acid (2TMS)]	55	0.352	0.481	8.774	0.409	30	112	25	117	17	119 duplicate
14447	131 [626; 5-Methylthioadeno	Phenylalanine	55	0.333	0.302	32.835	0.463	31	111	37	105	116	94 duplicate
17175	131 [626; 5-Methylthioadeno	Citric acid	55	0.316	0.311	33.973	0.523	32	110	38	108	117	55 duplicate
15050	131 [626; 5-Methylthioadeno	[548; Leucine (2TBS)]	52	0.300	0.489	16.408	0.499	33	109	23	119	57	76 duplicate
11025	131 [626; 5-Methylthioadeno	Isoleucine	47	0.295	0.217	26.369	0.360	34	108	40	102	97	133 duplicate
16636	131 [626; 5-Methylthioadeno	Glycerol-3-phosphate	55	0.282	0.182	31.472	0.530	35	107	43	99	113	50 duplicate
15975	131 [626; 5-Methylthioadeno	Glycerol-2-phosphate	55	0.255	0.503	7.782	0.408	36	106	21	121	12	121 duplicate
11157	131 [626; 5-Methylthioadeno	Proline	54	0.254	0.213	36.047	0.441	37	105	41	101	120	104 duplicate
18315	131 [626; 5-Methylthioadeno	9-(Z)-Octadecanoic acid	55	0.228	0.358	24.567	0.418	38	103	33	109	93	116 duplicate
14343	131 [626; 5-Methylthioadeno	[596; N-Acetylglutamic acid (2TMS)]	55	0.228	0.197	38.635	0.409	39	104	42	100	123	120 duplicate
13362	131 [626; 5-Methylthioadeno	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	46	0.227	0.538	10.943	0.477	40	102	19	123	28	88 duplicate
10073	131 [626; 5-Methylthioadeno	[938; Sulfuric acid (2TMS)]	29	0.222	0.146	13.390	0.449	41	101	46	86	42	100 duplicate
17101	131 [626; 5-Methylthioadeno	Glycetic acid-3-phosphate	55	0.211	0.271	12.478	0.453	42	100	38	104	35	98 duplicate
18601	131 [626; 5-Methylthioadeno	90 [910; 9-(Z)-Hexadecanoic acid (1TMS)]	55	0.196	0.324	16.268	0.403	43	99	35	107	55	124 duplicate
17731	131 [626; 5-Methylthioadeno	Lysine	55	0.166	0.105	48.924	0.408	44	98	50	92	138	122 duplicate
18621	131 [626; 5-Methylthioadeno	Trehalose	54	0.152	0.246	39.773	0.290	45	97	39	103	126	140 duplicate
19645	131 [626; 5-Methylthioadeno	[931; myo-Inositol-2-phosphate (7TMS)]	55	0.143	0.151	17.071	0.508	46	96	48	94	63	68 duplicate
10212	131 [626; 5-Methylthioadeno	2 Serine	53	0.141	0.151	27.088	0.384	47	95	44	98	101	129 duplicate
10892	131 [626; 5-Methylthioadeno	Threonine	55	0.138	0.124	39.919	0.418	48	94	47	85	127	117 duplicate
17530	131 [626; 5-Methylthioadeno	72 [919; D-Xylopyranose (4TMS)]	54	0.124	0.146	13.100	0.365	49	93	45	97	39	132 duplicate
8894	131 [626; 5-Methylthioadeno	Ergosterol	55	0.108	-0.002	23.487	0.441	50	92	56	86	91	105 original
19740	131 [626; 5-Methylthioadeno	[734; 1-Monooleoylglycerol (2TMS); 1-	50	0.105	0.116	9.138	0.359	51	91	49	83	21	134 duplicate
10487	131 [626; 5-Methylthioadeno	124 Monohexadecanoylglycerol (1TMS)]	44	0.095	0.095	41.810	0.312	52	90	52	90	130	138 duplicate
16473	131 [626; 5-Methylthioadeno	Phosphoric acid	55	0.095	0.101	26.163	0.349	53	89	51	91	96	136 duplicate
18280	131 [626; 5-Methylthioadeno	[636; 4R-Acetylido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane	53	0.081	-0.004	40.283	0.429	54	88	57	85	128	113 duplicate
19015	131 [626; 5-Methylthioadeno	58 (1TMS)]	33	0.053	-0.394	11.741	0.443	55	87	71	71	32	101 duplicate
18748	131 [626; 5-Methylthioadeno	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	51	0.018	0.034	8.756	0.436	56	86	54	88	16	107 duplicate
9898	131 [626; 5-Methylthioadeno	[607; Putrescine (4TMS)]	52	0.008	-0.167	9.124	0.502	57	85	60	82	19	72 original
17461	131 [626; 5-Methylthioadeno	Lanosta-8,24-dien-3-beta-ol	55	-0.003	-0.173	22.704	0.485	58	84	61	81	88	83 duplicate
9896	131 [626; 5-Methylthioadeno	[731; Erythrose (3TMS)]	30	-0.048	-0.027	6.930	0.297	59	83	58	84	8	139 original
18795	131 [626; 5-Methylthioadeno	[700; Ergosta-5,7-dien-3-ol]	55	-0.052	-0.557	31.768	0.588	60	82	85	57	114	25 duplicate
15432	131 [626; 5-Methylthioadeno	Hexadecanoic acid	55	-0.053	0.083	17.741	0.443	61	81	53	89	69	102 duplicate
19380	131 [626; 5-Methylthioadeno	[NA]	55	-0.068	-0.654	32.160	0.535	62	80	105	37	115	46 duplicate
9890	131 [626; 5-Methylthioadeno	Octadecanoic acid	55	-0.139	-0.267	16.990	0.454	63	79	64	78	61	97 original
18950	131 [626; 5-Methylthioadeno	[855; Squalene]	54	-0.147	-0.302	14.084	0.425	64	78	68	74	46	115 duplicate
19441	131 [626; 5-Methylthioadeno	111 [583; Tyramine (3TMS)]	35	-0.163	-0.387	7.164	0.491	65	77	69	73	10	81 duplicate
9895	131 [626; 5-Methylthioadeno	[583; Erythritol (4TMS)]	37	-0.168	-0.473	8.384	0.530	66	76	76	68	14	49 original

11928	131 [626; 5-Methylthioadenosine 15 Alanine	55 -0.180	-0.390	28.187	0.565	67	75	70	72	108	36 duplicate
9897	131 [626; 5-Methylthioadenosine 140 [892; Ergosta-7,22-dien-3-ol (1TMS)]	40 -0.182	-0.290	7.066	0.459	68	74	67	75	9	98 original
18930	131 [626; 5-Methylthioadenosine 97 [756; beta-D-Methylglucopyranoside (4TMS)]	44 -0.230	-0.252	30.032	0.530	69	73	63	79	110	48 duplicate
17985	131 [626; 5-Methylthioadenosine 79 Glucose	55 -0.269	-0.619	45.323	0.568	70	72	97	45	137	34 duplicate
19246	131 [626; 5-Methylthioadenosine 105 [705; 2-Ketogluconic acid (5TMS)]	41 -0.271	-0.272	20.867	0.568	71	71	65	77	80	35 duplicate
18651	131 [626; 5-Methylthioadenosine 91 [766; beta-D-Methylglucopyranoside (4TMS)]	55 -0.273	-0.231	23.805	0.487	72	70	62	80	82	82 duplicate
19823	131 [626; 5-Methylthioadenosine 118 [928; Glucopyranose-6-phosphate (6TMS)]	49 -0.282	-0.433	15.071	0.437	73	89	74	68	52	108 duplicate
18223	131 [626; 5-Methylthioadenosine 83 Sorbitol	51 -0.285	-0.161	30.809	0.354	74	68	59	83	112	135 duplicate
9892	131 [626; 5-Methylthioadenosine 135 [902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	55 -0.304	-0.515	22.846	0.435	75	67	78	64	87	109 original
18886	131 [626; 5-Methylthioadenosine 96 myo-Inositol	41 -0.315	-0.277	7.937	0.334	76	66	66	76	13	137 duplicate
19210	131 [626; 5-Methylthioadenosine 104 [795; Erythritol (4TMS)]	54 -0.317	-0.557	16.951	0.517	77	65	84	58	60	59 duplicate
19666	131 [626; 5-Methylthioadenosine 120 [945; Uridine (3TMS)]	45 -0.321	0.014	21.687	0.513	78	64	55	87	83	63 duplicate
18336	131 [626; 5-Methylthioadenosine 85 [528; Methylcitric acid (4TMS)]	42 -0.322	-0.672	12.935	0.514	79	63	108	34	36	62 duplicate
10758	131 [626; 5-Methylthioadenosine 6 Glycerol	55 -0.324	-0.578	51.170	0.573	80	62	89	53	141	32 duplicate
12300	131 [626; 5-Methylthioadenosine 18 [590; 1-Acetyl-2-thiohydantoin]	55 -0.340	-0.562	18.104	0.476	81	61	86	56	70	89 duplicate
19470	131 [626; 5-Methylthioadenosine 112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (8TMS)]	54 -0.358	-0.580	6.637	0.461	82	60	90	52	6	95 duplicate
11547	131 [626; 5-Methylthioadenosine 12 Glyceric acid	54 -0.360	-0.569	9.921	0.430	83	59	88	54	24	112 duplicate
19788	131 [626; 5-Methylthioadenosine 128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	38 -0.368	-0.547	18.470	0.500	84	58	83	59	73	74 duplicate
16390	131 [626; 5-Methylthioadenosine 57 [757; 2-Desoxy-pentose-3-ylose dimethoxyamine (2TMS)]	47 -0.369	-0.617	23.118	0.524	85	57	96	46	90	54 duplicate
17665	131 [626; 5-Methylthioadenosine 74 [912; Tetradecanoic acid (1TMS)]	55 -0.374	-0.743	17.317	0.538	86	56	127	15	64	45 duplicate
16082	131 [626; 5-Methylthioadenosine 54 [NA]	47 -0.382	-0.539	13.616	0.468	87	55	81	61	43	92 duplicate
19576	131 [626; 5-Methylthioadenosine 116 [882; Pseudouridine (5TMS)]	24 -0.384	-0.428	12.251	0.375	88	54	73	69	34	130 duplicate
18046	131 [626; 5-Methylthioadenosine 80 [772; D-Glucose (5TMS)]	54 -0.385	-0.610	41.495	0.540	89	53	94	48	129	43 duplicate
19785	131 [626; 5-Methylthioadenosine 127 [777; Fructose-6-phosphate methoxyamine (8TMS)]	32 -0.395	-0.402	14.237	0.401	91	51	72	70	47	125 duplicate
19135	131 [626; 5-Methylthioadenosine 102 [904; Galactose methoxyamine (5TMS)]	55 -0.407	-0.519	13.004	0.431	92	50	79	63	38	111 duplicate
14652	131 [626; 5-Methylthioadenosine 39 [829; 1-Phenylethanol (1TMS)]	54 -0.412	-0.670	26.465	0.511	93	49	107	35	98	65 duplicate
18445	131 [626; 5-Methylthioadenosine 87 [945; beta-D-Glucopyranose (5TMS)]	53 -0.414	-0.673	45.102	0.522	94	48	109	33	136	58 duplicate
12663	131 [626; 5-Methylthioadenosine 21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	55 -0.414	-0.542	27.132	0.476	95	46	82	60	102	80 duplicate
14853	131 [626; 5-Methylthioadenosine 41 [639; Proline (2TMS)]	55 -0.414	-0.709	24.648	0.574	96	47	117	25	94	31 duplicate
19756	131 [626; 5-Methylthioadenosine 125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	55 -0.415	-0.695	42.323	0.561	97	45	115	27	133	39 duplicate
15708	131 [626; 5-Methylthioadenosine 50 [746; Ribonic acid-1,4-lactone (3TMS)]	52 -0.416	-0.583	9.285	0.496	98	44	87	55	22	78 duplicate
19810	131 [626; 5-Methylthioadenosine 129 Glc]	50 -0.417	-0.652	19.771	0.593	99	43	102	40	76	20 duplicate
9893	131 [626; 5-Methylthioadenosine 136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	12 -0.424	-0.676	11.415	0.281	100	42	110	32	30	141 original
19098	131 [626; 5-Methylthioadenosine 101 [832; Dopamine (4TMS)]	55 -0.433	-0.438	19.793	0.509	101	41	75	67	77	68 duplicate
19723	131 [626; 5-Methylthioadenosine 123 [945; Galactofuranose-6-phosphate (7TMS)]	55 -0.436	-0.690	21.910	0.576	102	40	113	29	84	28 duplicate
18700	131 [626; 5-Methylthioadenosine 92 [680; Glycerol-2-phosphate (4TMS)]	47 -0.443	-0.624	17.379	0.500	103	39	99	43	65	75 duplicate
13587	131 [626; 5-Methylthioadenosine 29 Erythritol	55 -0.444	-0.606	14.730	0.527	104	38	92	50	50	51 duplicate
12422	131 [626; 5-Methylthioadenosine 19 Alanine (BP) (3TMS)	55 -0.453	-0.781	23.020	0.597	105	37	132	10	88	18 duplicate
12782	131 [626; 5-Methylthioadenosine 22 [690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	44 -0.461	-0.611	10.634	0.473	106	36	95	47	26	91 duplicate
19056	131 [626; 5-Methylthioadenosine 100 [857; Mannitol (6TMS)]	55 -0.468	-0.586	19.481	0.427	107	35	91	51	74	114 duplicate
15338	131 [626; 5-Methylthioadenosine 46 Arabinose	55 -0.476	-0.725	27.560	0.579	108	34	124	18	103	27 duplicate
17026	131 [626; 5-Methylthioadenosine 65 [646; 3-Deoxyglucitol (5TMS)]	54 -0.480	-0.716	19.954	0.575	109	33	120	22	78	30 duplicate
11675	131 [626; 5-Methylthioadenosine 13 Uracil	55 -0.481	-0.652	26.971	0.626	110	32	103	39	99	5 duplicate
12177	131 [626; 5-Methylthioadenosine 17 [700; 2-methyl-1,2-propanediol (2TMS)]	55 -0.488	-0.645	28.447	0.509	111	31	101	41	106	67 duplicate
18498	131 [626; 5-Methylthioadenosine 88 Gluconic acid	55 -0.490	-0.623	22.500	0.622	112	30	98	44	85	8 duplicate
19498	131 [626; 5-Methylthioadenosine 113 Galactose-6-phosphate	53 -0.491	-0.796	15.137	0.583	113	29	136	6	53	21 duplicate
9891	131 [626; 5-Methylthioadenosine 134 Isomaltose	55 -0.496	-0.724	35.373	0.608	114	28	123	19	119	14 original
19173	131 [626; 5-Methylthioadenosine 103 [648; Ethylamine (2TMS)]	54 -0.497	-0.530	23.079	0.516	115	27	80	62	89	60 duplicate

11418	131 [626; 5-Methylthioadeno 11	Succinic acid	55	-0.502	-0.652	18.333	0.442	116	25	104	38	71	103 duplicate
16308	131 [626; 5-Methylthioadeno 56	Orotic acid (3TMS)	55	-0.502	-0.713	17.451	0.584	117	26	119	23	66	26 duplicate
12053	131 [626; 5-Methylthioadeno 16	[644; 2-Methyl-1,3-butanediol (2TMS)]	55	-0.503	-0.643	28.533	-0.626	118	24	100	42	107	6 duplicate
18391	131 [626; 5-Methylthioadeno 86	[783; 2-Galactono-1,4-lactone (4TMS)]	52	-0.508	-0.754	30.798	0.607	119	23	129	13	111	13 duplicate
16795	131 [626; 5-Methylthioadeno 62	[812; D-Xylofuranose (4TMS)]	55	-0.511	-0.677	25.062	0.534	120	22	111	31	95	47 duplicate
13017	131 [626; 5-Methylthioadeno 24	[725; 2-Ketocacetic acid (2TMS)]	55	-0.512	-0.685	41.951	0.632	121	21	112	30	131	3 duplicate
15147	131 [626; 5-Methylthioadeno 44	[910; 2-Ketogluconic acid methoxymine (4TMS)]	48	-0.515	-0.717	19.584	0.564	122	20	122	20	75	37 duplicate
17391	131 [626; 5-Methylthioadeno 70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	48	-0.516	-0.607	28.272	0.537	123	19	93	49	104	44 duplicate
13248	131 [626; 5-Methylthioadeno 26	Citramalic acid	55	-0.518	-0.701	27.001	0.507	124	18	116	26	100	69 duplicate
14550	131 [626; 5-Methylthioadeno 38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	55	-0.523	-0.713	18.397	0.516	125	17	118	24	72	61 duplicate
19771	131 [626; 5-Methylthioadeno 126	[559; Erythritol (4TMS)]	38	-0.525	-0.792	14.262	0.591	126	16	134	8	48	22 duplicate
17923	131 [626; 5-Methylthioadeno 78	Mannose	53	-0.533	-0.744	16.722	0.569	127	15	128	14	59	33 duplicate
11802	131 [626; 5-Methylthioadeno 14	Fumaric acid	55	-0.537	-0.694	11.110	0.484	128	14	114	28	29	84 duplicate
14753	131 [626; 5-Methylthioadeno 40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	55	-0.538	-0.717	44.119	0.480	129	13	121	21	135	86 duplicate
17598	131 [626; 5-Methylthioadeno 73	[708; Glucose methoxymine (5TMS)]	49	-0.544	-0.763	15.929	0.499	130	12	131	11	54	77 duplicate
13475	131 [626; 5-Methylthioadeno 28	Malic acid	55	-0.556	-0.740	20.075	0.519	131	11	126	16	79	58 duplicate
19705	131 [626; 5-Methylthioadeno 122	[644; Erythritol (4TMS)]	44	-0.556	-0.729	13.759	0.508	132	10	125	17	45	70 duplicate
9889	131 [626; 5-Methylthioadeno 132	[895; Isomaltose methoxymine (8TMS)]	35	-0.556	-0.665	14.379	0.466	133	9	106	36	49	93 original
19686	131 [626; 5-Methylthioadeno 121	[657; Erythritol (4TMS)]	47	-0.563	-0.757	11.507	0.524	134	8	130	12	31	53 duplicate
19525	131 [626; 5-Methylthioadeno 114	Fructose-6-phosphate	44	-0.575	-0.824	13.265	0.597	135	7	140	2	41	19 duplicate
19281	131 [626; 5-Methylthioadeno 106	[733; Threitol (4TMS)]	53	-0.591	-0.794	20.868	0.614	136	6	135	7	81	10 duplicate
19411	131 [626; 5-Methylthioadeno 110	[715; Erythritol (4TMS)]	47	-0.593	-0.806	17.070	0.576	137	5	137	5	62	29 duplicate
19600	131 [626; 5-Methylthioadeno 117	[724; Glyceral (3TMS)]	49	-0.595	-0.787	18.395	0.503	138	4	133	9	56	71 duplicate
17796	131 [626; 5-Methylthioadeno 76	Fructose	55	-0.630	-0.817	36.218	0.605	139	3	139	3	121	15 duplicate
14238	131 [626; 5-Methylthioadeno 35	Pyroglutamic acid	55	-0.635	-0.810	50.713	0.588	140	2	138	4	140	24 duplicate
19551	131 [626; 5-Methylthioadeno 115	Glucose-6-phosphate	53	-0.668	-0.829	35.270	0.551	141	1	141	1	118	42 duplicate
19577	132 [895; Isomaltose metho 116	[882; Pseudouridine (5TMS)]	20	0.874	0.699	7.713	0.439	1	140	44	97	6	83 duplicate
18337	132 [895; Isomaltose metho 85	[528; Methylcitric acid (4TMS)]	27	0.864	0.849	14.163	0.374	2	139	21	120	42	108 duplicate
19471	132 [895; Isomaltose metho 112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	42	0.659	0.754	10.888	0.489	3	138	34	107	19	63 duplicate
19136	132 [895; Isomaltose metho 102	[904; Galactose methoxymine (5TMS)]	42	0.654	0.753	12.789	0.563	4	137	35	106	31	41 duplicate
9901	132 [895; Isomaltose metho 135	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	42	0.624	0.698	20.267	0.461	5	136	45	96	85	73 original
14239	132 [895; Isomaltose metho 35	Pyroglutamic acid	42	0.600	0.735	43.940	0.575	6	135	41	100	140	32 duplicate
9906	132 [895; Isomaltose metho 140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	33	0.595	0.738	9.381	0.407	7	134	40	101	12	98 original
13476	132 [895; Isomaltose metho 28	Malic acid	42	0.584	0.937	17.725	0.578	8	133	2	139	73	30 duplicate
17666	132 [895; Isomaltose metho 74	[912; Tetradecanoic acid (1TMS)]	42	0.577	0.713	13.090	0.421	9	132	42	99	35	93 duplicate
11803	132 [895; Isomaltose metho 14	Fumaric acid	42	0.570	0.911	10.990	0.585	10	131	5	138	20	27 duplicate
19552	132 [895; Isomaltose metho 115	Glucose-6-phosphate	42	0.568	0.762	30.590	0.610	11	130	32	109	118	19 duplicate
12783	132 [895; Isomaltose metho 22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	36	0.552	0.936	7.739	0.645	12	129	3	138	7	3 duplicate
13249	132 [895; Isomaltose metho 26	Citramalic acid	42	0.547	0.798	23.519	0.526	13	128	26	115	98	53 duplicate
19667	132 [895; Isomaltose metho 120	[945; Uridine (3TMS)]	40	0.538	0.309	20.043	0.572	14	127	79	62	83	33 duplicate
14754	132 [895; Isomaltose metho 40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	42	0.521	0.791	37.737	0.540	15	126	28	113	134	48 duplicate
12664	132 [895; Isomaltose metho 21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	42	0.517	0.741	23.791	0.531	16	125	39	102	100	52 duplicate
16798	132 [895; Isomaltose metho 62	[812; D-Xylofuranose (4TMS)]	42	0.515	0.851	21.814	0.615	17	123	20	121	95	15 duplicate
19057	132 [895; Isomaltose metho 100	[857; Mannitol (6TMS)]	42	0.515	0.832	17.243	0.564	18	124	23	118	72	37 duplicate
18887	132 [895; Isomaltose metho 96	myo-Inositol	31	0.497	0.516	10.842	0.297	19	122	59	82	18	126 duplicate
9905	132 [895; Isomaltose metho 139	[700; Ergosta-5,7-dien-3-ol]	25	0.493	0.419	11.510	0.476	20	121	69	72	23	67 original
11419	132 [895; Isomaltose metho 11	Succinic acid	42	0.487	0.859	16.553	0.597	21	120	18	123	63	22 duplicate
19282	132 [895; Isomaltose metho 106	[733; Threitol (4TMS)]	42	0.484	0.762	16.754	0.618	22	119	33	108	68	13 duplicate
17797	132 [895; Isomaltose metho 76	Fructose	42	0.477	0.781	31.304	0.591	23	118	29	112	119	25 duplicate
19757	132 [895; Isomaltose metho 125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	42	0.466	0.635	37.008	0.541	24	117	50	91	133	46 duplicate

11548	132 [895; Isomaltose metho]	12	Glycic acid	42	0.454	0.885	10.081	0.610	25	116	10	131	14	20 duplicate
19772	132 [895; Isomaltose metho]	128	[559; Erythritol (4TMS)]	38	0.440	0.654	8.822	0.548	26	115	47	94	10	45 duplicate
19708	132 [895; Isomaltose metho]	122	[844; Erythritol (4TMS)]	40	0.433	0.840	5.981	0.563	27	114	22	119	3	40 duplicate
12301	132 [895; Isomaltose metho]	18	[590; 1-Acetyl-2-thiohydantoin]	42	0.431	0.524	16.611	0.431	28	113	58	83	64	85 duplicate
9907	132 [895; Isomaltose metho]	141	Lanosta-8,24-dien-3-beta-ol	39	0.425	0.475	10.262	0.447	29	112	61	80	15	77 original
19646	132 [895; Isomaltose metho]	119	[931; myo-Inositol-2-phosphate (7TMS)]	42	0.412	0.399	14.948	0.459	30	111	74	67	49	74 duplicate
15339	132 [895; Isomaltose metho]	46	Arabinose	42	0.405	0.882	22.172	0.653	31	110	11	130	96	2 duplicate
19601	132 [895; Isomaltose metho]	117	[724; Glycerol (3TMS)]	40	0.403	0.750	11.481	0.533	32	109	37	104	22	51 duplicate
15148	132 [895; Isomaltose metho]	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	39	0.401	0.751	13.174	0.572	33	108	36	105	36	34 duplicate
19381	132 [895; Isomaltose metho]	109	Octadecanoic acid	42	0.386	0.470	27.594	0.390	34	107	63	78	114	101 duplicate
9804	132 [895; Isomaltose metho]	138	[674; Ergosterol (1TMS)]	33	0.394	0.377	10.337	0.376	35	106	76	65	16	108 original
19412	132 [895; Isomaltose metho]	110	[715; Erythritol (4TMS)]	39	0.387	0.746	9.821	0.629	36	105	38	103	13	9 duplicate
17824	132 [895; Isomaltose metho]	78	Mannose	40	0.387	0.692	12.301	0.564	37	104	46	95	28	38 duplicate
19442	132 [895; Isomaltose metho]	111	[583; Erythritol (4TMS)]	34	0.387	0.395	12.599	0.340	38	103	75	68	29	117 duplicate
16063	132 [895; Isomaltose metho]	54	[NA]	41	0.385	0.795	8.685	0.594	39	102	27	114	9	23 duplicate
13018	132 [895; Isomaltose metho]	24	[725; 2-Ketooctanoic acid (2TMS)]	42	0.380	0.897	36.685	0.622	40	101	8	133	132	12 duplicate
18392	132 [895; Isomaltose metho]	86	[793; D-Galactono-1,4-lactone (4TMS)]	39	0.379	0.861	25.471	0.659	41	100	17	124	108	1 duplicate
14551	132 [895; Isomaltose metho]	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	42	0.377	0.940	16.047	0.393	42	99	1	140	60	7 duplicate
17599	132 [895; Isomaltose metho]	73	[708; Glucose methoxyamine (5TMS)]	35	0.371	0.851	12.960	0.393	43	98	48	83	34	100 duplicate
18499	132 [895; Isomaltose metho]	88	Glucuronic acid	42	0.370	0.828	18.518	0.577	44	96	24	117	75	31 duplicate
18796	132 [895; Isomaltose metho]	94	Hexadecanoic acid	42	0.370	0.457	26.991	0.426	45	97	65	76	111	89 duplicate
12423	132 [895; Isomaltose metho]	19	Alanine (BP) (3TMS)	42	0.368	0.503	19.970	0.441	46	95	60	81	82	82 duplicate
12054	132 [895; Isomaltose metho]	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	42	0.368	0.878	24.689	0.612	47	94	13	128	101	17 duplicate
9803	132 [895; Isomaltose metho]	137	Ergosterol	42	0.361	0.118	20.734	0.350	48	93	84	57	88	114 original
17027	132 [895; Isomaltose metho]	65	[646; 3-Deoxyglucitol (5TMS)]	42	0.354	0.902	12.939	0.645	49	91	7	134	33	4 duplicate
19499	132 [895; Isomaltose metho]	113	Galactose-6-phosphate	42	0.354	0.578	12.803	0.494	50	92	54	87	32	62 duplicate
14854	132 [895; Isomaltose metho]	41	[639; Proline (2TMS)]	42	0.347	0.415	21.473	0.423	51	90	72	69	92	82 duplicate
18526	132 [895; Isomaltose metho]	114	Fructose-6-phosphate	40	0.346	0.603	10.525	0.487	52	89	53	88	17	64 duplicate
13588	132 [895; Isomaltose metho]	29	Erythritol	42	0.345	0.867	13.913	0.589	53	88	16	125	40	26 duplicate
15709	132 [895; Isomaltose metho]	50	[748; Ribonic acid-1,4-lactone (3TMS)]	42	0.343	0.855	8.837	0.591	54	87	19	122	11	24 duplicate
17392	132 [895; Isomaltose metho]	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	36	0.337	0.407	25.589	0.420	55	86	73	68	107	94 duplicate
19811	132 [895; Isomaltose metho]	129	Glc	41	0.329	0.881	13.676	0.630	56	85	12	129	39	8 duplicate
9900	132 [895; Isomaltose metho]	134	Isomaltose	42	0.329	0.907	30.496	0.638	57	84	6	135	117	6 original
16307	132 [895; Isomaltose metho]	56	[829; Orotic acid (3TMS)]	42	0.326	0.875	12.004	0.626	58	83	14	127	24	11 duplicate
16391	132 [895; Isomaltose metho]	57	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	41	0.324	0.870	16.629	0.617	59	82	15	126	65	14 duplicate
11676	132 [895; Isomaltose metho]	13	Uracil	42	0.319	0.889	22.855	0.611	60	81	9	132	97	18 duplicate
19687	132 [895; Isomaltose metho]	121	[657; Erythritol (4TMS)]	37	0.315	0.558	7.542	0.568	61	80	57	84	5	35 duplicate
19799	132 [895; Isomaltose metho]	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	37	0.285	0.709	12.655	0.579	62	79	43	98	30	29 duplicate
14653	132 [895; Isomaltose metho]	39	[829; 1-Phenylethanol (1TMS)]	42	0.282	0.927	21.627	0.626	63	78	4	137	93	10 duplicate
19724	132 [895; Isomaltose metho]	123	[945; Galactofuranose-6-phosphate (7TMS)]	42	0.277	0.317	19.197	0.446	64	77	78	63	79	79 duplicate
19786	132 [895; Isomaltose metho]	107	[777; Fructose-6-phosphate methoxyamine (6TMS)]	35	0.278	0.822	8.415	0.582	65	76	25	116	8	28 duplicate
12178	132 [895; Isomaltose metho]	17	[700; 2-methyl-1,2-propanediol (2TMS)]	42	0.275	0.766	24.696	0.562	66	75	31	110	102	42 duplicate
19602	132 [895; Isomaltose metho]	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	42	0.273	0.365	15.149	0.386	67	74	77	64	52	104 duplicate
9899	132 [895; Isomaltose metho]	133	[855; Squalene]	42	0.268	0.082	16.374	0.349	68	73	85	56	62	115 original
19316	132 [895; Isomaltose metho]	107	9-(Z)-Octadecenoic acid	42	0.259	0.158	21.309	0.378	69	72	83	58	91	105 duplicate
18224	132 [895; Isomaltose metho]	83	Sorbitol	37	0.246	-0.225	27.343	0.212	70	71	94	47	113	139 duplicate
9902	132 [895; Isomaltose metho]	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	15	0.219	0.420	2.964	0.376	71	70	68	73	1	107 original
18701	132 [895; Isomaltose metho]	92	[680; Glycerol-2-phosphate (4TMS)]	39	0.201	0.560	12.500	0.555	72	69	56	85	28	43 duplicate
18446	132 [895; Isomaltose metho]	87	[845; beta-D-Glucopyranose (5TMS)]	40	0.195	0.610	39.028	0.549	73	68	52	89	136	44 duplicate



19174	132 [895; Isomaltose metho]	103 [848; Ethylamine (2TMS)]	42 0,189	0,820	18,909	0,429	74	67	51	90	77	87 duplicate
18281	132 [895; Isomaltose metho]	84 Mannitol	40 0,172	0,416	35,653	0,417	75	66	70	71	131	96 duplicate
19741	132 [895; Isomaltose metho]	124 Monohexadecanoylglycerol (1TMS)]	38 0,169	-0,015	15,093	0,417	76	65	87	54	51	95 duplicate
19211	132 [895; Isomaltose metho]	104 [795; Erythritol (4TMS)]	41 0,151	0,259	15,579	0,450	77	64	81	60	57	76 duplicate
17462	132 [895; Isomaltose metho]	71 [731; Erythrose (3TMS)]	42 0,138	-0,086	20,408	0,443	78	63	93	48	86	80 duplicate
18652	132 [895; Isomaltose metho]	91 [766; beta-D-Methylglucopyranoside (4TMS)]	42 0,103	0,435	20,745	0,338	79	62	67	74	89	118 duplicate
19097	132 [895; Isomaltose metho]	101 [832; Dopamine (4TMS)]	42 0,092	0,450	17,087	0,329	80	60	68	75	69	121 duplicate
11929	132 [895; Isomaltose metho]	15 Alanine	42 0,092	-0,084	25,815	0,517	81	61	92	49	109	58 duplicate
10759	132 [895; Isomaltose metho]	6 Glycerol	42 0,089	0,472	43,854	0,540	82	59	62	79	139	48 duplicate
19247	132 [895; Isomaltose metho]	105 [705; 2-Ketogluconic acid (5TMS)]	38 0,058	0,651	14,764	0,471	83	58	49	92	48	68 duplicate
10074	132 [895; Isomaltose metho]	1 [938; Sulfuric acid (2TMS)]	32 0,056	0,565	6,661	0,567	84	57	55	86	4	36 duplicate
18931	132 [895; Isomaltose metho]	97 [756; beta-D-Methylglucopyranoside (4TMS)]	39 0,053	0,469	24,745	0,429	85	56	64	77	103	88 duplicate
18047	132 [895; Isomaltose metho]	80 [772; D-Glucose (5TMS)]	40 0,049	0,416	35,102	0,484	86	55	71	70	128	65 duplicate
19624	132 [895; Isomaltose metho]	118 [928; Glucopyranose-6-phosphate (6TMS)]	41 0,044	-0,078	14,315	0,436	87	54	90	51	43	84 duplicate
19016	132 [895; Isomaltose metho]	99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	33 0,042	0,772	4,239	0,604	88	53	30	111	2	21 duplicate
19349	132 [895; Isomaltose metho]	108 Octadecenoic acid	42 0,041	-0,230	14,162	0,467	89	52	95	46	41	69 duplicate
16951	132 [895; Isomaltose metho]	64 [789; Tyramine (3TMS)]	42 0,015	-0,020	14,576	0,371	90	51	88	53	46	111 duplicate
17531	132 [895; Isomaltose metho]	72 [919; D-Xylopyranose (4TMS)]	41 0,007	-0,081	14,700	0,359	91	50	91	50	47	112 duplicate
16637	132 [895; Isomaltose metho]	60 Glycerol-3-phosphate	42 0,006	-0,262	27,107	0,386	92	49	96	45	112	103 duplicate
17986	132 [895; Isomaltose metho]	79 Glucose	42 -0,015	0,293	38,559	0,519	93	48	80	61	135	56 duplicate
17176	132 [895; Isomaltose metho]	67 Citric acid	42 -0,080	-0,390	29,081	0,327	94	47	99	42	116	122 duplicate
15433	132 [895; Isomaltose metho]	47 [NA]	42 -0,094	0,041	17,234	0,504	95	46	86	55	71	60 duplicate
15976	132 [895; Isomaltose metho]	53 Glycerol-2-phosphate	42 -0,106	-0,033	12,315	0,271	96	45	89	52	27	132 duplicate
14448	132 [895; Isomaltose metho]	37 Phenylalanine	42 -0,110	-0,502	28,331	0,348	97	44	106	35	115	116 duplicate
18749	132 [895; Isomaltose metho]	93 [607; Putrescine (4TMS)]	41 -0,115	0,237	12,093	0,292	98	43	82	59	25	127 duplicate
10893	132 [895; Isomaltose metho]	7 Threonine	42 -0,131	-0,434	34,042	0,283	99	42	101	40	126	129 duplicate
18822	132 [895; Isomaltose metho]	130 Trehalose	42 -0,134	-0,330	33,775	0,411	100	41	97	44	125	97 duplicate
15888	132 [895; Isomaltose metho]	52 [NA]	28 -0,138	-0,439	15,522	0,533	101	40	103	38	55	50 duplicate
14344	132 [895; Isomaltose metho]	36 [596; N-Acetylglutamic acid (2TMS)]	42 -0,187	-0,451	32,825	0,332	102	39	104	37	123	119 duplicate
16474	132 [895; Isomaltose metho]	58 [1TMS)]	42 -0,203	-0,416	23,832	0,282	103	38	100	41	99	130 duplicate
13918	132 [895; Isomaltose metho]	32 [729; N,N-Dimethyllysine methyl ester]	41 -0,229	-0,738	21,144	0,462	104	37	126	15	90	72 duplicate
13699	132 [895; Isomaltose metho]	30 [815; Ethyl-3(2H)-thiophenone]	42 -0,231	-0,584	33,011	0,284	105	36	115	28	124	128 duplicate
17321	132 [895; Isomaltose metho]	69 Arginine	38 -0,232	-0,816	26,803	0,517	106	35	131	10	110	57 duplicate
10351	132 [895; Isomaltose metho]	3 Ethanolamine	40 -0,238	-0,594	14,973	0,423	107	34	117	24	50	91 duplicate
10213	132 [895; Isomaltose metho]	2 Serine	40 -0,246	-0,513	25,726	0,245	108	33	108	33	108	136 duplicate
17732	132 [895; Isomaltose metho]	75 Lysine	42 -0,250	-0,503	41,153	0,314	109	31	107	34	137	124 duplicate
18107	132 [895; Isomaltose metho]	81 Tyrosine	42 -0,250	-0,678	35,454	0,525	110	32	125	16	129	54 duplicate
10488	132 [895; Isomaltose metho]	4 Phosphoric acid	30 -0,251	-0,384	34,933	0,217	111	30	98	43	127	136 duplicate
14026	132 [895; Isomaltose metho]	33 Methionine	42 -0,252	-0,600	19,467	0,371	112	29	119	22	80	110 duplicate
16717	132 [895; Isomaltose metho]	61 [NA]	42 -0,259	-0,527	15,707	0,454	113	28	109	32	58	75 duplicate
16874	132 [895; Isomaltose metho]	63 Glutamine	36 -0,289	-0,561	15,815	0,614	114	27	112	29	59	16 duplicate
14133	132 [895; Isomaltose metho]	34 Aspartic acid	42 -0,284	-0,563	35,591	0,352	115	26	113	28	130	113 duplicate
11158	132 [895; Isomaltose metho]	9 Proline	41 -0,302	-0,555	31,578	0,242	116	25	110	31	120	137 duplicate
17102	132 [895; Isomaltose metho]	66 Glycetic acid-3-phosphate	42 -0,303	-0,638	15,192	0,481	117	24	122	19	53	66 duplicate
17861	132 [895; Isomaltose metho]	77 benzeneacetic acid methyl ester]	41 -0,305	-0,615	32,607	0,330	118	23	121	20	122	120 duplicate
16556	132 [895; Isomaltose metho]	59 Ornithine; Arginine	42 -0,326	-0,608	41,917	0,372	119	22	120	21	138	109 duplicate
14953	132 [895; Isomaltose metho]	42 Glutamic acid	38 -0,334	-0,658	32,261	0,317	120	21	123	18	121	123 duplicate
18188	132 [895; Isomaltose metho]	82 Lysine	20 -0,337	-0,848	19,045	0,446	121	20	135	6	78	78 duplicate

11026	132 [895; Isomaltose metho]	8	Isoleucine	33	-0.348	-0.436	25.272	0.127	122	19	102	39	105	140 duplicate
16149	132 [895; Isomaltose metho]	55	[612; 4-Aminobutyric acid (2TBS)]	23	-0.375	-0.585	14.566	0.280	123	18	116	25	45	131 duplicate
13809	132 [895; Isomaltose metho]	31	[622; Parabanic acid (2TMS)]	42	-0.384	-0.739	15.558	0.517	124	17	127	14	56	59 duplicate
13363	132 [895; Isomaltose metho]	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	31	-0.406	-0.844	21.662	0.441	125	16	134	7	84	81 duplicate
12901	132 [895; Isomaltose metho]	23	Homoserine	42	-0.412	-0.868	20.087	0.503	126	15	136	5	84	81 duplicate
18842	132 [895; Isomaltose metho]	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	28	-0.413	-0.495	13.608	0.252	127	14	105	36	38	135 duplicate
15051	132 [895; Isomaltose metho]	43	[548; Leucine (2TBS)]	38	-0.425	-0.557	17.894	0.312	128	13	111	30	74	125 duplicate
15244	132 [895; Isomaltose metho]	45	Homocysteine	39	-0.428	-0.565	16.130	0.406	129	12	114	27	61	99 duplicate
11289	132 [895; Isomaltose metho]	10	Glycine	42	-0.429	-0.912	25.040	0.640	130	11	140	1	104	5 duplicate
15618	132 [895; Isomaltose metho]	49	[877; Pyrophosphoric acid (4TMS)]	42	-0.433	-0.595	18.553	0.463	131	10	118	23	76	71 duplicate
15799	132 [895; Isomaltose metho]	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	24	-0.478	-0.742	15.309	0.388	132	9	128	13	54	102 duplicate
18551	132 [895; Isomaltose metho]	89	[775; Dopamine (4TMS)]	20	-0.505	-0.792	17.024	0.430	133	8	130	11	67	88 duplicate
18974	132 [895; Isomaltose metho]	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	28	-0.508	-0.882	17.024	0.525	134	7	137	4	68	55 duplicate
13134	132 [895; Isomaltose metho]	25	[708; 2,5-Diaminovalerolactam (2TMS)]	38	-0.514	-0.909	20.489	0.564	135	6	139	2	87	39 duplicate
15526	132 [895; Isomaltose metho]	48	Asparagine	42	-0.515	-0.835	19.589	0.541	136	5	133	8	81	47 duplicate
10624	132 [895; Isomaltose metho]	5	Leucine	25	-0.527	-0.758	17.231	0.258	137	4	129	12	70	134 duplicate
18832	132 [895; Isomaltose metho]	131	[626; 5-Methylthiadenosine (3TMS)]	35	-0.556	-0.665	14.379	0.466	138	3	124	17	44	70 duplicate
12544	132 [895; Isomaltose metho]	20	[619; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	14	-0.560	-0.832	13.222	0.424	139	2	132	9	37	90 duplicate
17249	132 [895; Isomaltose metho]	68	[570; Hypoxanthine (2TMS)]	10	-0.689	-0.908	11.426	0.262	140	1	138	3	21	133 duplicate
9912	133 [855; Squalene]	138	[674; Ergosterol (1TMS)]	46	0.627	0.832	15.921	0.606	1	141	1	141	77	1 original
18338	133 [855; Squalene]	85	[529; Methylcitric acid (4TMS)]	48	0.571	0.725	4.014	0.571	2	140	2	140	2	3 duplicate
19382	133 [855; Squalene]	109	Octadecanoic acid	64	0.560	0.664	18.389	0.411	3	139	5	137	98	35 duplicate
19578	133 [855; Squalene]	116	[882; Pseudouridine (5TMS)]	30	0.549	0.450	8.784	0.387	4	138	13	129	21	60 duplicate
17667	133 [855; Squalene]	74	[912; Tetradecanoic acid (1TMS)]	64	0.477	0.537	8.853	0.513	5	137	7	135	23	4 duplicate
9911	133 [855; Squalene]	137	Ergosterol	64	0.473	0.715	9.881	0.416	6	136	3	139	28	27 original
18797	133 [855; Squalene]	94	Hexadecanoic acid	64	0.467	0.682	17.865	0.494	7	135	4	138	92	6 duplicate
9915	133 [855; Squalene]	141	Lanosta-8,24-dien-3-beta-ol	61	0.463	0.609	13.504	0.494	8	134	6	136	57	5 original
9914	133 [855; Squalene]	140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	49	0.461	0.516	16.510	0.573	9	133	9	133	88	2 original
18927	133 [855; Squalene]	114	Fructose-6-phosphate	53	0.435	0.426	8.588	0.416	10	132	15	127	20	25 duplicate
18225	133 [855; Squalene]	83	Sorbitol	58	0.425	0.250	17.965	0.390	11	131	42	100	93	55 duplicate
19500	133 [855; Squalene]	113	Galactose-6-phosphate	62	0.383	0.243	9.637	0.416	12	130	43	89	27	26 duplicate
18212	133 [855; Squalene]	104	[795; Erythritol (4TMS)]	63	0.355	0.380	7.115	0.428	13	129	25	117	6	19 duplicate
19725	133 [855; Squalene]	123	[945; Galactofuranose-6-phosphate (7TMS)]	64	0.325	0.390	8.357	0.422	14	128	22	120	19	21 duplicate
19742	133 [855; Squalene]	124	[734; 1-Monooleoylglycerol (2TMS); 1-	59	0.309	0.523	23.031	0.355	15	127	8	134	117	115 duplicate
9910	133 [855; Squalene]	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.309	0.497	3.635	0.314	16	126	11	131	1	139 original
19443	133 [855; Squalene]	111	[583; Erythritol (4TMS)]	42	0.303	0.507	18.309	0.397	17	125	10	132	104	49 duplicate
12424	133 [855; Squalene]	19	Alanine (BP) (3TMS)	64	0.302	0.361	8.603	0.436	18	124	30	112	25	16 duplicate
9913	133 [855; Squalene]	139	[700; Ergosta-5,7-dien-3-ol]	38	0.300	0.399	18.112	0.486	19	123	17	125	102	7 original
14755	133 [855; Squalene]	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.299	0.287	31.886	0.377	20	122	37	105	135	77 duplicate
14855	133 [855; Squalene]	41	[639; Proline (2TMS)]	64	0.297	0.395	10.943	0.443	21	121	19	123	38	13 duplicate
17600	133 [855; Squalene]	73	[708; Glucose methoxyamine (5TMS)]	57	0.286	0.391	10.481	0.376	22	120	21	121	34	81 duplicate
18553	133 [855; Squalene]	115	Glucose-6-phosphate	62	0.279	0.218	22.223	0.340	23	119	51	91	115	128 duplicate
17463	133 [855; Squalene]	71	[731; Erythrose (3TMS)]	64	0.273	0.370	9.633	0.416	24	118	27	115	26	24 duplicate
12302	133 [855; Squalene]	18	[590; 1-Acetyl-2-thiohydantoin]	64	0.270	0.326	6.407	0.365	25	117	32	110	4	97 duplicate
13477	133 [855; Squalene]	28	Malic acid	64	0.269	0.172	7.767	0.381	26	116	60	82	16	71 duplicate
19773	133 [855; Squalene]	126	[559; Erythritol (4TMS)]	45	0.269	0.391	8.212	0.404	27	115	20	122	18	38 duplicate
18842	133 [855; Squalene]	132	[895; Isomaltose methoxyamine (8TMS)]	42	0.268	0.082	16.374	0.349	28	114	77	65	85	123 duplicate
14240	133 [855; Squalene]	35	Pyroglutamic acid	64	0.251	0.165	38.757	0.360	29	113	62	80	140	105 duplicate
17798	133 [855; Squalene]	76	Fructose	64	0.243	0.186	23.390	0.365	30	112	56	86	118	99 duplicate

19688	133 [855; Squalene]	121 [657; Erythritol (4TMS)]	55	0.239	0.288	14.176	0.360	31	111	36	106	64	106 duplicate
19137	133 [855; Squalene]	102 [904; Galactose methoxyamine (5TMS)]	64	0.232	0.223	7.429	0.420	32	110	50	92	13	23 duplicate
17925	133 [855; Squalene]	78 Mannose	62	0.226	0.239	11.889	0.413	33	109	45	97	47	31 duplicate
13250	133 [855; Squalene]	26 Citramalic acid	64	0.223	0.241	13.846	0.365	34	108	44	88	62	96 duplicate
19707	133 [855; Squalene]	122 [644; Erythritol (4TMS)]	52	0.219	0.227	15.864	0.412	35	107	47	95	74	32 duplicate
19058	133 [855; Squalene]	100 [857; Mannitol (6TMS)]	64	0.214	0.135	7.618	0.380	36	106	67	75	15	72 duplicate
19283	133 [855; Squalene]	106 [733; Threitol (4TMS)]	62	0.214	0.224	10.689	0.406	37	105	48	93	35	37 duplicate
19758	133 [855; Squalene]	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	0.208	0.110	29.709	0.357	38	104	73	69	129	111 duplicate
11604	133 [855; Squalene]	14 Fumaric acid	64	0.207	0.133	9.934	0.378	39	103	69	73	29	76 duplicate
14345	133 [855; Squalene]	36 [596; N-Acetylglutamic acid (2TMS)]	64	0.199	0.368	25.746	0.384	40	102	28	114	122	63 duplicate
16638	133 [855; Squalene]	60 Glycerol-3-phosphate	64	0.198	0.382	18.611	0.385	41	100	24	118	98	62 duplicate
12665	133 [855; Squalene]	21 [878; N,N-Di-(2-hydroxyethyl)-methanamine (2TMS)]	64	0.198	0.149	14.249	0.378	42	101	65	77	65	74 duplicate
17177	133 [855; Squalene]	67 Citric acid	64	0.192	0.294	21.164	0.359	43	99	35	107	110	108 duplicate
19413	133 [855; Squalene]	110 [715; Erythritol (4TMS)]	54	0.191	0.185	12.994	0.401	44	98	57	85	55	42 duplicate
19602	133 [855; Squalene]	117 [724; Glyceral (3TMS)]	56	0.188	0.226	9.602	0.402	45	97	48	94	24	41 duplicate
19317	133 [855; Squalene]	107 9-(Z)-Octadecenoic acid	64	0.185	0.432	11.742	0.363	46	96	14	128	45	102 duplicate
17393	133 [855; Squalene]	70 [893; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	0.184	0.134	15.651	0.384	47	95	68	74	71	101 duplicate
16952	133 [855; Squalene]	64 [789; Tyramine (3TMS)]	63	0.184	0.215	6.302	0.365	48	94	52	90	3	95 duplicate
15149	133 [855; Squalene]	44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	50	0.182	0.209	10.250	0.379	49	93	55	87	33	73 duplicate
17987	133 [855; Squalene]	79 Glucose	64	0.179	0.214	32.348	0.375	50	92	53	89	136	83 duplicate
19823	133 [855; Squalene]	130 Trehalose	63	0.174	0.307	27.413	0.382	51	91	34	108	125	69 duplicate
12784	133 [855; Squalene]	22 [690; N,N-Di-(2-hydroxyethyl)-methanamine (2TMS)]	52	0.172	0.122	12.762	0.383	52	90	71	71	53	67 duplicate
19647	133 [855; Squalene]	119 [931; myo-Inositol-2-phosphate (7TMS)]	64	0.171	0.310	7.225	0.335	53	88	33	109	8	134 duplicate
16475	133 [855; Squalene]	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	0.168	0.285	13.517	0.402	55	87	39	103	58	40 duplicate
17733	133 [855; Squalene]	75 Lysine	64	0.163	0.362	36.891	0.382	56	86	29	113	138	70 duplicate
19472	133 [855; Squalene]	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.158	0.156	18.903	0.404	57	85	64	78	87	39 duplicate
10894	133 [855; Squalene]	7 Threonine	64	0.158	0.399	27.414	0.421	58	84	18	124	126	22 duplicate
16797	133 [855; Squalene]	82 [812; D-Xylofuranose (4TMS)]	64	0.147	0.055	12.086	0.389	59	83	83	59	49	57 duplicate
18393	133 [855; Squalene]	66 [783; D-Galactono-1,4-lactone (4TMS)]	61	0.138	0.105	21.541	0.384	60	82	74	68	111	64 duplicate
19350	133 [855; Squalene]	108 Octadecenoic acid	64	0.132	0.386	7.403	0.360	61	81	23	119	12	104 duplicate
14552	133 [855; Squalene]	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.129	0.042	7.815	0.376	62	80	86	56	17	80 duplicate
14449	133 [855; Squalene]	37 Phenylalanine	64	0.124	0.371	20.020	0.414	63	79	26	116	107	29 duplicate
9909	133 [855; Squalene]	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64	0.118	0.181	10.000	0.456	64	78	58	84	31	8 original
11930	133 [855; Squalene]	15 Alanine	64	0.112	0.117	16.301	0.349	65	76	72	70	82	122 duplicate
11420	133 [855; Squalene]	11 Succinic acid	64	0.112	0.056	7.351	0.354	66	77	82	60	11	118 duplicate
19668	133 [855; Squalene]	120 [945; Uridine (3TMS)]	54	0.100	-0.084	11.010	0.398	67	75	114	28	39	47 duplicate
10760	133 [855; Squalene]	6 Glycerol	64	0.097	0.057	39.302	0.373	68	74	81	61	141	88 duplicate
15710	133 [855; Squalene]	50 [746; Ribonic acid-1,4-lactone (3TMS)]	61	0.096	0.014	18.999	0.433	69	73	89	53	100	17 duplicate
19625	133 [855; Squalene]	118 [928; Glucopyranose-6-phosphate (6TMS)]	58	0.091	0.049	10.154	0.357	70	72	85	57	32	110 duplicate
18888	133 [855; Squalene]	96 myo-Inositol	49	0.088	-0.034	19.870	0.316	71	71	104	38	106	138 duplicate
19812	133 [855; Squalene]	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	59	0.059	0.053	13.308	0.377	72	70	84	58	56	76 duplicate
11549	133 [855; Squalene]	129 Gic	63	0.054	-0.024	12.126	0.354	73	69	101	41	50	117 duplicate
18500	133 [855; Squalene]	88 Gluconic acid	64	0.054	0.002	12.275	0.401	74	68	94	48	51	44 duplicate
13589	133 [855; Squalene]	29 Erythritol	64	0.052	-0.047	7.220	0.411	75	67	106	36	7	33 duplicate
17028	133 [855; Squalene]	65 [846; 3-Deoxyglucitol (5TMS)]	63	0.044	0.031	15.854	0.351	76	66	88	54	73	120 duplicate
9908	133 [855; Squalene]	134 Isomaltose	64	0.043	0.011	24.002	0.365	77	65	91	51	119	98 original
17103	133 [855; Squalene]	68 Glycerc acid-3-phosphate	64	0.040	0.266	7.264	0.411	78	62	41	101	9	34 duplicate
18603	133 [855; Squalene]	90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	64	0.040	0.160	6.993	0.326	79	63	63	79	5	138 duplicate

15340	133 [855; Squalene]	46	Arabinose	64	0.040	0.014	17.967	0.369	80	64	90	52	94	90 duplicate
10214	133 [855; Squalene]	2	Serine	62	0.038	0.425	15.904	0.388	81	60	16	126	76	59 duplicate
18447	133 [855; Squalene]	87	[945; beta-D-Glucopyranose (5TMS)]	62	0.038	0.077	32.814	0.374	82	61	78	64	137	84 duplicate
19787	133 [855; Squalene]	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	39	0.036	-0.027	7.559	0.278	83	59	103	39	14	141 duplicate
16308	133 [855; Squalene]	56	[829; Uridic acid (3TMS)]	64	0.036	-0.010	13.641	0.351	84	58	98	46	59	119 duplicate
11677	133 [855; Squalene]	13	Uracil	64	0.035	-0.022	15.287	0.433	85	57	100	42	69	18 duplicate
18108	133 [855; Squalene]	81	Tyrosine	64	0.033	0.212	31.328	0.415	86	56	84	88	134	28 duplicate
13019	133 [855; Squalene]	24	[725; 2-Ketobutanoic acid (2TMS)]	64	0.031	-0.022	29.971	0.395	87	55	99	43	131	51 duplicate
16557	133 [855; Squalene]	59	Omithine; Arginine	64	0.028	0.168	36.320	0.364	88	54	61	81	139	100 duplicate
17862	133 [855; Squalene]	77	benzaneacetic acid methyl ester	62	0.019	0.228	27.077	0.367	89	53	48	96	124	94 duplicate
14654	133 [855; Squalene]	39	[829; 1-Phenylethanol (1TMS)]	63	0.018	0.001	16.339	0.362	90	52	95	47	83	103 duplicate
12055	133 [855; Squalene]	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	0.017	-0.053	16.193	0.439	91	51	109	33	80	15 duplicate
18975	133 [855; Squalene]	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	48	0.014	0.072	18.269	0.337	92	50	79	63	95	130 duplicate
10352	133 [855; Squalene]	3	Ethanolamine	62	0.013	0.132	11.565	0.346	93	49	70	72	44	125 duplicate
18702	133 [855; Squalene]	92	[680; Glyceral-2-phosphate (4TMS)]	54	0.012	-0.011	10.697	0.298	94	48	97	45	36	140 duplicate
18048	133 [855; Squalene]	80	[772; D-Glucose (5TMS)]	62	0.009	0.009	28.795	0.336	95	47	92	60	128	133 duplicate
16392	133 [855; Squalene]	57	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	55	0.005	0.032	15.040	0.340	96	46	87	55	68	127 duplicate
14954	133 [855; Squalene]	42	Glutamic acid	60	0.002	0.286	26.991	0.374	97	45	38	104	123	87 duplicate
12179	133 [855; Squalene]	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	0.000	-0.049	16.300	0.368	98	44	107	35	81	91 duplicate
16064	133 [855; Squalene]	54	[NA]	55	-0.010	-0.078	14.021	0.359	99	43	112	30	63	107 duplicate
11159	133 [855; Squalene]	9	Proline	63	-0.011	0.342	24.474	0.388	100	42	31	111	120	45 duplicate
19175	133 [855; Squalene]	103	[648; Ethylamine (2TMS)]	63	-0.017	-0.213	16.340	0.385	101	41	123	19	84	61 duplicate
13810	133 [855; Squalene]	31	[622; Parabanic acid (2TMS)]	64	-0.028	0.139	11.182	0.374	102	40	66	76	42	85 duplicate
10489	133 [855; Squalene]	4	Phosphoric acid	51	-0.031	0.277	29.710	0.369	103	39	40	102	130	58 duplicate
17532	133 [855; Squalene]	72	[919; D-Xylopyranose (4TMS)]	61	-0.031	-0.134	11.019	0.357	104	38	117	25	40	113 duplicate
13364	133 [855; Squalene]	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	-0.061	-0.041	19.107	0.368	105	37	105	37	101	92 duplicate
13919	133 [855; Squalene]	32	[729; N,N-Dimethyllysine methyl ester]	63	-0.065	0.178	15.828	0.447	106	36	59	83	72	10 duplicate
15977	133 [855; Squalene]	53	Glycerol-2-phosphate	64	-0.067	-0.167	11.888	0.383	107	35	121	21	46	66 duplicate
19800	133 [855; Squalene]	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	-0.069	-0.151	9.958	0.337	108	34	119	23	30	129 duplicate
16718	133 [855; Squalene]	61	[NA]	64	-0.077	-0.084	7.349	0.337	109	33	113	29	10	131 duplicate
11027	133 [855; Squalene]	8	Isoleucine	55	-0.079	0.457	15.316	0.414	110	32	12	130	70	30 duplicate
13700	133 [855; Squalene]	30	[815; Ethyl-3(2H)-thiophenone]	64	-0.085	0.087	27.500	0.378	111	31	76	66	127	75 duplicate
14027	133 [855; Squalene]	33	Methionine	64	-0.091	0.062	10.860	0.398	112	30	80	62	37	46 duplicate
17322	133 [855; Squalene]	69	Arginine	60	-0.093	0.007	19.294	0.394	113	29	93	49	103	54 duplicate
11290	133 [855; Squalene]	10	Glycine	64	-0.109	-0.051	17.240	0.384	114	28	108	34	90	65 duplicate
19098	133 [855; Squalene]	101	[832; Dopamine (4TMS)]	64	-0.110	-0.372	13.706	0.389	115	27	133	9	60	58 duplicate
14134	133 [855; Squalene]	34	Aspartic acid	64	-0.116	-0.020	30.468	0.355	116	26	98	44	132	116 duplicate
19017	133 [855; Squalene]	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	-0.129	-0.068	11.989	0.424	117	25	110	32	48	20 duplicate
18653	133 [855; Squalene]	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	-0.138	-0.392	20.227	0.401	118	24	136	6	109	43 duplicate
19833	133 [855; Squalene]	131	[626; 5-Methylthioadenosine (3TMS)]	55	-0.139	-0.071	11.396	0.397	120	23	126	16	88	9 duplicate
12802	133 [855; Squalene]	23	Homoserine	64	-0.140	-0.071	11.396	0.397	120	22	111	31	43	50 duplicate
18932	133 [855; Squalene]	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	-0.145	-0.306	21.920	0.377	121	21	130	12	113	79 duplicate
19800	133 [855; Squalene]	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.152	-0.025	20.126	0.395	122	20	102	40	108	52 duplicate
18843	133 [855; Squalene]	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	-0.166	-0.112	18.802	0.350	123	19	115	27	99	121 duplicate
19248	133 [855; Squalene]	105	[705; 2-Ketogluconic acid (5TMS)]	48	-0.168	-0.331	14.430	0.411	124	18	131	11	67	36 duplicate
12545	133 [855; Squalene]	20	[618; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.170	-0.365	15.894	0.441	125	17	132	10	75	14 duplicate
15527	133 [855; Squalene]	48	Asparagine	64	-0.171	-0.140	12.821	0.368	126	16	118	24	54	93 duplicate
15052	133 [855; Squalene]	43	[548; Leucine (2TBS)]	60	-0.182	-0.270	8.809	0.347	127	15	127	15	22	124 duplicate

18282	133 [855; Squalene]	84	Mannitol	62	-0.185	-0.432	30.813	0.383	128	14	139	3	133	68 duplicate
15245	133 [855; Squalene]	45	Homocysteine	61	-0.208	-0.253	21.957	0.341	129	13	125	17	114	126 duplicate
15889	133 [855; Squalene]	52	[NA]	46	-0.241	-0.152	19.369	0.394	130	12	120	22	105	53 duplicate
17250	133 [855; Squalene]	68	[570; Hypoxanthine (2TMS)]	20	-0.253	-0.240	14.320	0.318	131	11	124	18	66	137 duplicate
18750	133 [855; Squalene]	93	[607; Putrescine (4TMS)]	60	-0.258	-0.404	18.490	0.358	132	10	137	5	97	109 duplicate
13135	133 [855; Squalene]	25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.262	-0.117	16.050	0.338	133	8	118	26	78	132 duplicate
16150	133 [855; Squalene]	55	[612; 4-Aminobutyric acid (2TBS)]	43	-0.285	-0.381	23.022	0.375	134	8	135	7	116	82 duplicate
15434	133 [855; Squalene]	47	[NA]	64	-0.280	-0.417	13.761	0.397	135	7	138	4	61	48 duplicate
15619	133 [855; Squalene]	49	[677; Pyrophosphoric acid (4TMS)]	64	-0.291	-0.294	21.644	0.374	136	6	129	13	112	88 duplicate
10075	133 [855; Squalene]	1	[938; Sulfuric acid (2TMS)]	36	-0.292	-0.373	11.128	0.370	137	5	134	8	41	89 duplicate
16875	133 [855; Squalene]	63	Glutamine	52	-0.317	-0.185	17.148	0.334	138	4	122	20	89	135 duplicate
18552	133 [855; Squalene]	89	[775; Dopamine (4TMS)]	35	-0.355	-0.286	17.768	0.356	139	3	128	14	91	114 duplicate
18167	133 [855; Squalene]	82	Lysine	39	-0.377	-0.578	16.092	0.446	140	2	141	1	79	11 duplicate
10825	133 [855; Squalene]	5	Leucine	45	-0.418	-0.504	12.474	0.445	141	1	140	2	52	12 duplicate
134 Isomaltose														
16393	134 Isomaltose	57	[757; 2-Deoxy-pentose-3-yose dimethoxyamine (2TMS)]	55	0.868	0.983	17.015	0.718	1	141	6	136	31	7 duplicate
17029	134 Isomaltose	65	[646; 3-Deoxyglucitol (5TMS)]	63	0.850	0.993	22.503	0.734	2	140	1	141	62	2 duplicate
134 Isomaltose														
18913	134 Isomaltose	129	Glc	59	0.850	0.981	20.448	0.693	3	139	7	135	54	13 duplicate
15341	134 Isomaltose	46	Arabinose	64	0.850	0.990	11.265	0.734	4	138	3	139	9	3 duplicate
11678	134 Isomaltose	13	Urecl	64	0.843	0.983	9.580	0.710	5	137	5	137	5	8 duplicate
16309	134 Isomaltose	56	[829; Orotic acid (3TMS)]	64	0.840	0.980	23.225	0.727	6	136	2	140	71	4 duplicate
13020	134 Isomaltose	24	[725; 2-Ketooctanoic acid (2TMS)]	64	0.835	0.988	12.002	0.738	7	135	4	138	12	1 duplicate
12056	134 Isomaltose	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	0.829	0.973	9.602	0.710	8	134	9	133	6	9 duplicate
18394	134 Isomaltose	86	[783; D-Galactone-1,4-lactone (4TMS)]	61	0.807	0.980	9.385	0.726	9	133	8	134	3	5 duplicate
15711	134 Isomaltose	50	[746; Ribonic acid-1,4-lactone (3TMS)]	61	0.777	0.954	37.125	0.623	10	132	12	130	135	44 duplicate
18501	134 Isomaltose	88	Gluconic acid	64	0.765	0.933	15.005	0.688	11	131	16	126	18	15 duplicate
12180	134 Isomaltose	17	[700; 2-methyl-1,2-propanediol (2TMS)]	64	0.763	0.928	9.493	0.615	12	130	18	124	4	52 duplicate
16065	134 Isomaltose	55	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	55	0.762	0.947	28.391	0.628	13	129	13	129	107	43 duplicate
19018	134 Isomaltose	39	[629; 1-Phenylethanol (1TMS)]	63	0.755	0.967	11.019	0.693	14	128	17	125	98	25 duplicate
14655	134 Isomaltose	29	Erythritol	64	0.755	0.938	23.288	0.643	15	127	10	132	8	14 duplicate
13590	134 Isomaltose	92	[680; Glycerol-2-phosphate (4TMS)]	54	0.753	0.839	22.885	0.619	17	125	36	108	67	47 duplicate
18703	134 Isomaltose	62	[812; D-Xylofuranose (4TMS)]	64	0.737	0.939	13.835	0.662	18	124	14	128	15	26 duplicate
14553	134 Isomaltose	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.711	0.956	19.223	0.674	19	123	11	131	47	20 duplicate
19176	134 Isomaltose	103	[648; Ethylamine (2TMS)]	63	0.711	0.857	16.987	0.590	20	122	30	112	30	61 duplicate
19249	134 Isomaltose	105	[705; 2-Ketogluconic acid (5TMS)]	48	0.707	0.896	18.888	0.658	21	121	25	117	45	30 duplicate
18933	134 Isomaltose	11	Succinic acid	64	0.693	0.904	19.519	0.616	22	120	23	119	49	49 duplicate
11421	134 Isomaltose	97	[756; beta-D-Methylglucopyranoside (4TMS)]	52	0.676	0.838	11.925	0.585	23	119	37	105	11	63 duplicate
18055	134 Isomaltose	14	Fumaric acid	64	0.631	0.925	27.848	0.645	24	118	19	123	102	37 duplicate
11550	134 Isomaltose	12	Glyceric acid	63	0.605	0.850	29.922	0.602	25	117	32	110	110	57 duplicate
17789	134 Isomaltose	76	Fructose	64	0.601	0.917	6.307	0.681	26	116	21	121	1	18 duplicate
17926	134 Isomaltose	78	Mannose	62	0.599	0.851	24.439	0.597	27	115	31	111	81	58 duplicate
13478	134 Isomaltose	28	Malic acid	64	0.593	0.918	18.003	0.658	28	114	20	122	40	29 duplicate
12785	134 Isomaltose	52	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.593	0.902	28.247	0.639	29	113	24	118	105	40 duplicate
18654	134 Isomaltose	91	[766; beta-D-Methylglucopyranoside (4TMS)]	64	0.585	0.713	20.027	0.492	30	112	52	90	51	98 duplicate
17394	134 Isomaltose	70	[693; 2-Furan-2-hydroxyacetic acid (4TMS)]	57	0.584	0.654	10.731	0.564	31	111	58	84	7	76 duplicate
19801	134 Isomaltose	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	45	0.584	0.879	19.503	0.651	32	110	28	114	48	34 duplicate
19099	134 Isomaltose	101	[832; Dopamine (4TMS)]	64	0.581	0.757	19.615	0.534	33	109	46	98	50	81 duplicate
19284	134 Isomaltose	106	[733; Threitol (4TMS)]	62	0.579	0.880	17.796	0.695	34	108	27	115	36	12 duplicate
17601	134 Isomaltose	73	[708; Glucose methoxyamine (5TMS)]	57	0.568	0.784	21.599	0.546	35	107	40	102	58	74 duplicate



9920	134 Isomaltose	139 [700; Ergosta-5,7-dien-3-ol]	38	-0.084	-0.159	34.246	0.446	87	55	87	55	123	117 original
16876	134 Isomaltose	63 Glutamine	52	-0.106	-0.755	35.281	0.698	88	54	122	20	128	11 duplicate
19648	134 Isomaltose	119 [931; myo-Inositol-2-phosphate (7TMS)]	64	-0.112	-0.185	24.068	0.536	89	53	79	89	80 duplicate	
15053	134 Isomaltose	43 [548; Leucine (2TBS)]	60	-0.123	-0.379	22.845	0.491	90	52	97	45	63	88 duplicate
19318	134 Isomaltose	107 9-(Z)-Octadecenoic acid	64	-0.130	-0.305	17.805	0.420	91	51	83	49	37	129 duplicate
17533	134 Isomaltose	72 [919; D-Xylopyranose (4TMS)]	63	-0.133	-0.160	28.085	0.329	92	50	88	54	103	140 duplicate
9918	134 Isomaltose	138 [674; Ergosterol (1TMS)]	46	-0.150	0.022	33.832	0.457	93	49	83	59	122	112 original
9918	134 Isomaltose	137 Ergosterol	64	-0.159	-0.200	21.518	0.483	94	48	90	52	57	86 original
9917	134 Isomaltose	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17	-0.162	-0.372	16.063	0.508	95	47	98	46	23	93 original
17464	134 Isomaltose	71 [731; Erythrose (3TMS)]	64	-0.212	-0.274	18.478	0.456	96	48	91	51	43	113 duplicate
19743	134 Isomaltose	[734; 1-Monooleoylglycerol (2TMS); 1-Monoheptadecenoylethanol (1TMS)]	59	-0.218	-0.350	43.125	0.417	97	45	95	47	140	130 duplicate
10490	134 Isomaltose	4 Phosphoric acid	51	-0.227	-0.416	22.198	0.330	98	44	98	44	59	139 duplicate
15890	134 Isomaltose	52 [NA]	46	-0.233	-0.671	37.719	0.668	99	43	112	30	136	24 duplicate
19824	134 Isomaltose	130 Trehalose	63	-0.251	-0.331	17.555	0.398	100	42	94	48	35	133 duplicate
13136	134 Isomaltose	25 [709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.284	-0.904	35.226	0.658	101	41	136	6	127	31 duplicate
16476	134 Isomaltose	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	-0.290	-0.434	20.353	0.389	102	40	89	43	52	134 duplicate
16719	134 Isomaltose	61 [NA]	64	-0.305	-0.508	25.197	0.513	103	39	100	42	88	87 duplicate
19351	134 Isomaltose	108 Octadecanoic acid	64	-0.329	-0.518	28.325	0.410	104	38	101	41	106	131 duplicate
17734	134 Isomaltose	75 Lysine	64	-0.336	-0.539	25.719	0.440	105	37	102	40	90	121 duplicate
13365	134 Isomaltose	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53	-0.337	-0.800	36.081	0.574	106	36	124	18	131	87 duplicate
18976	134 Isomaltose	98 [697; Ribose-5-phosphate methoxamine (5TMS)]	48	-0.344	-0.794	36.217	0.563	107	35	123	19	132	68 duplicate
12903	134 Isomaltose	23 Homoserine	64	-0.377	-0.837	28.531	0.622	108	34	129	13	108	45 duplicate
10895	134 Isomaltose	7 Threonine	64	-0.385	-0.561	18.777	0.409	109	33	104	38	44	132 duplicate
15620	134 Isomaltose	49 [877; Pyrophosphoric acid (4TMS)]	64	-0.393	-0.595	41.322	0.480	110	32	106	36	138	104 duplicate
15246	134 Isomaltose	45 Homocysteine	61	-0.396	-0.611	41.494	0.440	111	31	107	35	139	120 duplicate
14346	134 Isomaltose	36 [596; N-Acetylglutamic acid (2TMS)]	64	-0.397	-0.588	20.434	0.438	112	30	105	37	53	122 duplicate
17251	134 Isomaltose	68 [570; Hypoxanthine (2TMS)]	20	-0.411	-0.928	23.356	0.592	113	29	138	4	73	60 duplicate
10215	134 Isomaltose	2 Serine	62	-0.435	-0.623	26.283	0.430	114	28	108	34	93	126 duplicate
17104	134 Isomaltose	66 Glycine acid-3-phosphate	64	-0.453	-0.650	27.752	0.476	115	27	111	31	100	107 duplicate
18944	134 Isomaltose	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50	-0.460	-0.686	36.036	0.520	116	26	115	27	130	83 duplicate
18553	134 Isomaltose	89 [775; Dopamine (4TMS)]	35	-0.466	-0.869	29.980	0.589	117	25	133	9	111	62 duplicate
11028	134 Isomaltose	8 Isoleucine	55	-0.476	-0.555	22.815	0.341	118	24	103	39	68	138 duplicate
14135	134 Isomaltose	34 Aspartic acid	64	-0.476	-0.643	23.024	0.501	119	23	109	33	68	94 duplicate
13811	134 Isomaltose	31 [622; Parabanic acid (2TMS)]	64	-0.487	-0.730	32.392	0.537	120	22	120	22	117	78 duplicate
19834	134 Isomaltose	131 [626; 5-Methylthioadenosine (3TMS)]	55	-0.496	-0.724	35.373	0.606	121	21	118	24	129	54 duplicate
14450	134 Isomaltose	37 Phenylalanine	64	-0.506	-0.727	16.818	0.477	122	20	119	23	29	106 duplicate
17178	134 Isomaltose	67 Citric acid	64	-0.515	-0.672	16.158	0.452	123	19	113	29	24	114 duplicate
11160	134 Isomaltose	9 Proline	63	-0.519	-0.674	27.804	0.427	124	18	114	28	101	127 duplicate
15528	134 Isomaltose	48 Asparagine	64	-0.525	-0.862	30.038	0.671	125	17	131	11	112	23 duplicate
14028	134 Isomaltose	33 Methionine	64	-0.535	-0.714	28.200	0.514	126	16	116	26	104	84 duplicate
16639	134 Isomaltose	60 Glycerol-3-phosphate	64	-0.541	-0.649	17.551	0.513	127	15	110	32	34	89 duplicate
15801	134 Isomaltose	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.556	-0.832	33.301	0.514	128	14	127	15	121	85 duplicate
13701	134 Isomaltose	30 [815; Ethyl-3(2H)-thiophenone]	64	-0.592	-0.724	24.595	0.435	129	13	117	25	83	123 duplicate
13920	134 Isomaltose	32 [729; N,N-Dimethyllysine methyl ester]	63	-0.611	-0.844	37.125	0.618	130	12	130	12	134	48 duplicate
17323	134 Isomaltose	69 Arginine	60	-0.617	-0.904	24.728	0.649	131	11	135	7	85	35 duplicate
16558	134 Isomaltose	59 Ornithine; Arginine	64	-0.618	-0.744	27.442	0.492	132	10	121	21	99	97 duplicate
10353	134 Isomaltose	3 Ethanolamine	62	-0.634	-0.863	32.699	0.605	133	9	132	10	120	55 duplicate
12546	134 Isomaltose	20 [619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.647	-0.948	23.512	0.672	134	8	139	3	74	22 duplicate

10626	134 isomaltose	5	Leucine	45	-0.648	-0.814	23,630	0.529	135	7	125	17	77	82	64	17
16151	134 isomaltose	55	[612; 4-Aminobutyric acid (2TBS)]	43	-0.650	-0.874	34,329	0.583	136	6	134	8	124	64	17	65
18168	134 isomaltose	82	Lysine	39	-0.673	-0.970	22,809	0.682	137	5	141	1				
			[626; beta-[[[5-methyl-2-thienyl)methyl]enylamino]-													
			benzeneacetic acid methyl ester]													
77	benzeneacetic acid methyl ester]	77	benzeneacetic acid methyl ester]	62	-0.674	-0.835	27,116	0.485	138	4	128	14	98	102	64	102
42	Glutamic acid	42	Glutamic acid	60	-0.685	-0.817	29,200	0.489	139	3	128	16	109	101	64	101
10	Glycine	64	-0.689	64	-0.689	-0.966	22,757	0.720	140	2	140	2	64	6	17	64
81	Tyrosine	64	-0.732	64	-0.732	-0.918	27,261	0.661	141	1	137	5	97	28	64	28
112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63	0.754	0.909	23,665	0.586	1	141	1	141	121	1	1	1
102	[904; Galactose methoxymine (5TMS)]	102	[904; Galactose methoxymine (5TMS)]	30	0.713	0.842	12,168	0.572	2	140	2	140	47	2	47	2
116	[882; Pseudoouridine (5TMS)]	116	[882; Pseudoouridine (5TMS)]	30	0.692	0.777	11,914	0.345	3	139	4	138	43	38	43	38
100	[857; Mannitol (6TMS)]	100	[857; Mannitol (6TMS)]	64	0.842	0.801	5,059	0.533	4	138	3	139	8	6	8	6
132	[895; Isomaltose methoxymine (8TMS)]	132	[895; Isomaltose methoxymine (8TMS)]	42	0.624	0.696	20,267	0.461	5	137	11	131	102	53	102	53
12	Glyceric acid	63	0.544	63	0.544	0.720	17,708	0.487	6	136	9	133	87	30	87	30
28	Malic acid	64	0.544	64	0.544	0.754	4,406	0.526	7	135	6	136	3	7	136	3
126	[559; Erythritol (4TMS)]	126	[559; Erythritol (4TMS)]	45	0.533	0.695	12,353	0.516	8	134	12	130	49	11	49	11
22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	52	0.519	0.737	18,246	0.475	9	133	8	134	90	44	90	44
115	Glucose-6-phosphate	62	0.506	62	0.506	0.523	14,334	0.483	10	132	39	103	65	37	65	37
111	[583; Erythritol (4TMS)]	42	0.494	42	0.494	0.668	25,691	0.447	11	131	16	126	131	66	131	66
11	Succinic acid	64	0.488	64	0.488	0.672	6,483	0.463	12	129	15	127	13	52	13	52
35	Pyrogulamic acid	64	0.488	64	0.488	0.503	30,437	0.454	13	130	47	95	138	60	138	60
44	[910; 2-Ketogluconic acid methoxymine (4TMS)]	50	0.486	50	0.486	0.630	10,411	0.493	14	128	21	121	33	26	33	26
40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	64	0.474	64	0.474	0.702	15,545	0.469	15	127	10	132	75	50	75	50
121	[657; Erythritol (4TMS)]	55	0.469	55	0.469	0.603	20,132	0.459	17	125	26	116	100	55	100	55
122	[644; Erythritol (4TMS)]	58	0.461	58	0.461	0.754	8,200	0.548	19	123	5	137	18	8	18	8
85	[529; Methylcitric acid (4TMS)]	64	0.457	64	0.457	0.657	10,176	0.503	20	122	18	124	32	20	32	20
29	Erythritol	64	0.457	64	0.457	0.690	4,737	0.472	21	121	13	129	6	48	13	48
21	Citramalic acid	64	0.452	64	0.452	0.690	4,737	0.472	21	121	13	129	6	48	13	48
26	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64	0.449	64	0.449	0.654	5,650	0.485	22	119	20	122	11	2	18	13
62	[812; D-Xylofuranose (4TMS)]	62	[812; D-Xylofuranose (4TMS)]	64	0.449	0.584	3,645	0.507	23	120	31	111	2	18	31	18
74	[912; Tetradecanoic acid (1TMS)]	64	0.448	64	0.448	0.740	14,123	0.475	24	118	7	135	62	46	62	46
110	[715; Erythritol (4TMS)]	54	0.438	54	0.438	0.572	16,456	0.500	25	117	33	109	81	21	109	81
128	[824; D-Scotoheptulose-7-phosphate (7TMS)]	128	[824; D-Scotoheptulose-7-phosphate (7TMS)]	45	0.430	0.622	7,863	0.439	26	116	23	119	16	70	119	16
117	[724; Glycerol (3TMS)]	56	0.426	56	0.426	0.625	12,927	0.515	27	115	22	120	54	12	120	54
76	Fructose	64	0.421	64	0.421	0.464	16,318	0.480	28	114	55	87	79	40	87	79
38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	63	0.420	63	0.420	0.584	7,306	0.484	29	113	14	128	15	34	14	34
54	[NA]	65	0.418	65	0.418	0.585	17,697	0.474	30	112	29	113	88	47	113	88
18	[590; 1-Acetyl-2-thiohydantoin]	64	0.410	64	0.410	0.609	6,639	0.420	31	111	25	117	14	83	117	14
106	[733; Threitol (4TMS)]	62	0.397	62	0.397	0.531	11,075	0.516	32	110	38	104	39	10	104	39
120	[945; Uridine (3TMS)]	54	0.391	54	0.391	0.169	5,092	0.473	33	109	79	63	9	46	79	63
113	Galactose-6-phosphate	62	0.387	62	0.387	0.452	14,420	0.403	34	108	58	84	67	92	84	67
96	myo-Inositol	49	0.366	49	0.366	0.440	25,601	0.331	35	107	59	83	130	140	130	140
24	[725; 2-Ketooctanoic acid (2TMS)]	64	0.381	64	0.381	0.574	21,476	0.510	37	105	32	110	109	15	109	15
24	[725; 2-Ketooctanoic acid (2TMS)]	64	0.381	64	0.381	0.511	14,567	0.398	38	104	43	99	70	99	99	70
114	Fructose-6-phosphate	53	0.376	53	0.376	0.542	8,701	0.449	39	103	37	105	23	65	105	23
127	[777; Fructose-6-phosphate methoxymine (6TMS)]	71	[777; Fructose-6-phosphate methoxymine (6TMS)]	64	0.373	0.409	2,141	0.495	40	102	62	80	1	23	80	1
71	[731; Erythrose (3TMS)]	64	0.374	64	0.374	0.316	12,373	0.390	41	101	69	73	50	106	73	50
92	[680; Glycerol-2-phosphate (4TMS)]	54	0.372	54	0.372	0.316	12,373	0.390	41	101	69	73	50	106	73	50
39	[829; 1-Phenylethanol (1TMS)]	63	0.370	63	0.370	0.614	12,009	0.478	42	100	24	118	45	41	118	45
16	[644; 2-Methyl-1,3-butanediol (2TMS)]	64	0.365	64	0.365	0.590	7,863	0.511	43	99	28	114	17	13	114	17
86	[793; D-Galactono-1,4-lactone (4TMS)]	61	0.352	61	0.352	0.507	18,452	0.540	44	98	45	97	93	5	97	93



17927	135 [902; Melibiose (8TMS); 78 Mannose	62	0.346	0.492	16,305	0.413	45	97	50	92	78	89 duplicate
16310	135 [902; Melibiose (8TMS); 56 [828; Orotic acid (3TMS)]	64	0.346	0.523	16,444	0.494	46	98	40	102	80	24 duplicate
17660	135 [902; Melibiose (8TMS); 125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64	0.338	0.316	22,003	0.409	47	95	68	74	112	90 duplicate
15342	135 [902; Melibiose (8TMS); 46 Arabinose	64	0.334	0.505	14,686	0.480	48	94	48	96	73	27 duplicate
19859	135 [902; Melibiose (8TMS); 134 Isomaltose	64	0.331	0.546	17,093	0.509	49	93	35	107	82	17 duplicate
19384	135 [902; Melibiose (8TMS); 109 Octadecanoic acid	64	0.330	0.585	14,231	0.386	50	92	30	112	64	110 duplicate
17030	135 [902; Melibiose (8TMS); 65 [646; 3-Deoxyglucitol (5TMS)]	63	0.326	0.553	18,050	0.499	51	91	34	108	89	22 duplicate
18799	135 [902; Melibiose (8TMS); 94 Hexadecanoic acid	64	0.323	0.594	11,661	0.450	52	90	27	115	40	64 duplicate
18502	135 [902; Melibiose (8TMS); 88 Gluconic acid	64	0.322	0.514	9,457	0.507	53	89	41	101	28	19 duplicate
12181	135 [902; Melibiose (8TMS); 17 [700; 2-methyl-1,2-propanediol (2TMS)]	64	0.320	0.513	8,664	0.418	54	88	42	100	22	88 duplicate
16394	135 [902; Melibiose (8TMS); 57 [757; 2-Desoxy-pentos-3-yose dimethoxyamine (2TMS)]	55	0.320	0.465	13,737	0.457	55	87	53	89	60	56 duplicate
18227	135 [902; Melibiose (8TMS); 83 Sorbitol	58	0.316	0.020	11,972	0.331	56	86	90	52	44	141 duplicate
18284	135 [902; Melibiose (8TMS); 84 Mannitol	62	0.301	0.321	21,924	0.414	57	85	67	75	111	88 duplicate
17602	135 [902; Melibiose (8TMS); 73 [708; Glucose methoxyamine (5TMS)]	57	0.301	0.483	15,085	0.382	58	84	51	91	74	115 duplicate
9927	135 [902; Melibiose (8TMS); 140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49	0.288	0.458	21,725	0.484	59	83	56	86	110	33 original
11679	135 [902; Melibiose (8TMS); 13 Uracil	64	0.284	0.545	8,656	0.510	60	82	36	106	21	14 duplicate
19250	135 [902; Melibiose (8TMS); 105 [705; 2-Ketogluconic acid (5TMS)]	48	0.278	0.465	11,050	0.475	61	81	54	88	38	43 duplicate
19814	135 [902; Melibiose (8TMS); 129 Glic	59	0.274	0.499	14,630	0.476	62	80	48	94	71	42 duplicate
15712	135 [902; Melibiose (8TMS); 50 [746; Ribonic acid-1,4-lactone (3TMS)]	61	0.273	0.509	25,764	0.435	63	79	44	98	132	73 duplicate
17395	135 [902; Melibiose (8TMS); 70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57	0.266	0.273	9,475	0.380	64	78	70	72	29	116 duplicate
19177	135 [902; Melibiose (8TMS); 103 [648; Ethylamine (2TMS)]	63	0.264	0.412	13,901	0.458	65	77	81	81	61	59 duplicate
9928	135 [902; Melibiose (8TMS); 141 Lanosta-8,24-dien-3-beta-ol	61	0.258	0.431	20,338	0.457	66	76	60	82	104	57 original
19019	135 [902; Melibiose (8TMS); 99 [662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	41	0.234	0.493	15,575	0.422	67	75	49	93	78	82 duplicate
12426	135 [902; Melibiose (8TMS); 19 Alanine (BP) (3TMS)	64	0.221	0.400	6,246	0.469	68	74	63	79	12	51 duplicate
9925	135 [902; Melibiose (8TMS); 138 [674; Ergosterol (1TMS)]	46	0.215	0.453	22,024	0.480	69	73	57	85	113	39 original
9924	135 [902; Melibiose (8TMS); 137 Ergosterol	64	0.192	0.206	9,023	0.386	70	72	75	67	25	112 original
18100	135 [902; Melibiose (8TMS); 101 [832; Dopamine (4TMS)]	64	0.190	0.266	12,053	0.385	71	71	72	70	46	113 duplicate
19727	135 [902; Melibiose (8TMS); 123 [945; Galactofuranose-6-phosphate (7TMS)]	64	0.189	0.270	4,463	0.428	72	70	71	71	5	80 duplicate
18934	135 [902; Melibiose (8TMS); 97 [756; beta-D-Methylglucopyranoside (4TMS)]	52	0.189	0.213	16,015	0.368	73	69	74	68	77	123 duplicate
18752	135 [902; Melibiose (8TMS); 93 [607; Putrescine (4TMS)]	60	0.179	0.142	23,155	0.372	74	68	81	61	117	120 duplicate
14857	135 [902; Melibiose (8TMS); 41 [639; Proline (2TMS)]	64	0.177	0.362	4,859	0.444	75	67	64	78	7	67 duplicate
18649	135 [902; Melibiose (8TMS); 119 [931; myo-Inositol-2-phosphate (7TMS)]	64	0.174	0.340	9,121	0.437	76	66	65	77	26	72 duplicate
18954	135 [902; Melibiose (8TMS); 64 [789; Tyramine (3TMS)]	63	0.164	0.177	10,659	0.486	77	65	78	64	38	31 duplicate
9923	135 [902; Melibiose (8TMS); 138 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.162	0.338	5,846	0.400	78	64	66	76	11	95 original
18655	135 [902; Melibiose (8TMS); 91 [766; beta-D-Methylglucopyranoside (4TMS)]	64	0.145	0.222	17,691	0.383	79	63	73	69	85	114 duplicate
19214	135 [902; Melibiose (8TMS); 104 [795; Erythritol (4TMS)]	63	0.125	0.191	10,868	0.391	80	62	76	66	37	104 duplicate
18952	135 [902; Melibiose (8TMS); 133 [855; Squalene]	64	0.118	0.181	10,000	0.456	81	61	77	65	31	58 duplicate
18605	135 [902; Melibiose (8TMS); 90 [910; 9-(Z)-Hexadecenoic acid (1TMS)]	64	0.108	0.132	8,216	0.393	82	60	82	60	19	103 duplicate
9926	135 [902; Melibiose (8TMS); 139 [700; Ergosta-5,7-dien-3-ol]	38	0.107	0.106	23,507	0.427	83	59	86	56	119	79 original
10762	135 [902; Melibiose (8TMS); 67 Glycerol	64	0.102	0.114	30,974	0.347	84	57	85	57	140	134 duplicate
19319	135 [902; Melibiose (8TMS); 107 9-(Z)-Octadecenoic acid	64	0.102	0.094	4,450	0.352	85	58	87	55	4	133 duplicate
11932	135 [902; Melibiose (8TMS); 15 Alanine	64	0.069	-0.016	9,353	0.469	86	56	93	49	27	49 duplicate
17179	135 [902; Melibiose (8TMS); 67 Citric acid	64	0.068	0.123	12,613	0.390	87	55	84	58	53	107 duplicate
16640	135 [902; Melibiose (8TMS); 60 Glycerol-3-phosphate	64	0.061	0.123	10,577	0.398	88	54	83	59	34	98 duplicate
19449	135 [902; Melibiose (8TMS); 87 [945; beta-D-Glucopyranose (5TMS)]	62	0.044	0.152	25,592	0.420	89	53	80	62	129	84 duplicate
14451	135 [902; Melibiose (8TMS); 37 Phenylalanine	64	0.026	-0.040	11,719	0.358	90	52	94	48	41	128 duplicate
18152	135 [902; Melibiose (8TMS); 55 [812; 4-Aminobutyric acid (2TBS)]	43	0.025	-0.131	27,189	0.387	91	51	97	45	134	109 duplicate
18744	135 [902; Melibiose (8TMS); 124 Monohexadecano/glycerol (2TMS)]	59	-0.015	-0.101	30,517	0.400	92	50	96	46	139	94 duplicate

18845	135 [902; Melibiose (8TMS); 95	[770; 3,4,6-Trisubstituted phenylmethanamine (5TMS)]	50	-0.019	-0.133	25.266	0.454	93	49	98	44	128	61 duplicate
17889	135 [902; Melibiose (8TMS); 79	Glucose	64	-0.027	0.063	24.518	0.389	94	48	89	53	124	108 duplicate
10077	135 [902; Melibiose (8TMS); 1	[938; Sulfuric acid (2TMS)]	36	-0.029	0.013	11.727	0.334	95	47	92	50	42	138 duplicate
10896	135 [902; Melibiose (8TMS); 7	Threonine	64	-0.044	-0.079	19.237	0.334	96	46	95	47	98	139 duplicate
16720	135 [902; Melibiose (8TMS); 61	[NA]	64	-0.051	0.069	9.553	0.371	97	45	88	54	30	121 duplicate
15691	135 [902; Melibiose (8TMS); 52	[NA]	46	-0.053	-0.167	24.589	0.440	98	44	101	41	125	68 duplicate
18050	135 [902; Melibiose (8TMS); 80	[772; D-Glucose (5TMS)]	62	-0.071	0.015	21.289	0.360	99	43	91	51	107	126 duplicate
15602	135 [902; Melibiose (8TMS); 51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44	-0.074	-0.319	25.223	0.487	100	42	116	26	127	29 duplicate
15436	135 [902; Melibiose (8TMS); 47	[NA]	64	-0.080	-0.219	13.526	0.425	101	41	104	38	57	81 duplicate
19352	135 [902; Melibiose (8TMS); 108	Octadecanoic acid	64	-0.103	-0.153	13.203	0.368	102	40	100	42	56	122 duplicate
10354	135 [902; Melibiose (8TMS); 3	Ethanolamine	62	-0.105	-0.204	17.385	0.415	103	39	102	40	83	87 duplicate
19627	135 [902; Melibiose (8TMS); 118	[928; Glucopyranose-6-phosphate (8TMS)]	58	-0.113	-0.148	14.377	0.394	104	38	99	43	66	102 duplicate
16110	135 [902; Melibiose (8TMS); 81	Tyrosine	64	-0.145	-0.271	24.129	0.428	105	37	107	35	123	78 duplicate
17864	135 [902; Melibiose (8TMS); 77	[826; beta-[[[5-methyl-2-thienyl]methyleneamino- benzeneacetic acid methyl ester]	62	-0.150	-0.235	20.951	0.356	106	36	105	37	105	129 duplicate
15979	135 [902; Melibiose (8TMS); 53	Glycerol-2-phosphate	64	-0.170	-0.327	17.740	0.394	107	35	117	25	88	101 duplicate
17252	135 [902; Melibiose (8TMS); 68	[570; Hypoxanthine (2TMS)]	20	-0.178	-0.651	18.439	0.399	108	34	138	4	92	96 duplicate
10827	135 [902; Melibiose (8TMS); 5	Leucine	45	-0.184	-0.518	14.445	0.484	109	33	135	7	68	35 duplicate
13702	135 [902; Melibiose (8TMS); 30	[815; Ethyl-3-(2H)-thiophenone]	64	-0.186	-0.280	20.323	0.347	110	32	112	30	103	135 duplicate
12547	135 [902; Melibiose (8TMS); 20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31	-0.191	-0.423	19.205	0.548	111	31	125	17	95	4 duplicate
17534	135 [902; Melibiose (8TMS); 72	[919; D-Xylopyranose (4TMS)]	63	-0.194	-0.288	14.675	0.365	112	30	110	32	72	124 duplicate
14136	135 [902; Melibiose (8TMS); 34	Aspartic acid	64	-0.212	-0.266	22.425	0.405	113	29	106	36	115	91 duplicate
15529	135 [902; Melibiose (8TMS); 48	Asparagine	64	-0.217	-0.372	13.544	0.460	114	28	122	20	58	54 duplicate
14029	135 [902; Melibiose (8TMS); 33	Methionine	64	-0.221	-0.354	12.343	0.440	115	27	121	21	48	69 duplicate
11029	135 [902; Melibiose (8TMS); 45	Isoleucine	55	-0.223	-0.336	13.557	0.355	116	26	118	24	59	130 duplicate
15247	135 [902; Melibiose (8TMS); 8	Homocysteine	61	-0.223	-0.338	28.629	0.378	117	25	119	23	135	117 duplicate
17324	135 [902; Melibiose (8TMS); 69	Arginine	60	-0.225	-0.517	14.134	0.516	118	24	134	8	63	9 duplicate
14347	135 [902; Melibiose (8TMS); 36	[596; N-Acetylglutamic acid (2TMS)]	64	-0.230	-0.273	18.299	0.378	119	23	108	34	91	119 duplicate
16877	135 [902; Melibiose (8TMS); 82	Glutamine	52	-0.237	-0.303	19.614	0.419	120	22	115	27	97	85 duplicate
18169	135 [902; Melibiose (8TMS); 63	Lysine	39	-0.242	-0.545	13.011	0.481	121	21	136	6	55	38 duplicate
17105	135 [902; Melibiose (8TMS); 66	Glyceric acid-3-phosphate	64	-0.259	-0.275	12.510	0.428	122	20	109	33	52	77 duplicate
11292	135 [902; Melibiose (8TMS); 10	Glycine	64	-0.271	-0.502	10.642	0.510	123	19	131	11	35	16 duplicate
14956	135 [902; Melibiose (8TMS); 42	Glutamic acid	60	-0.273	-0.439	22.077	0.398	124	18	127	15	114	100 duplicate
16559	135 [902; Melibiose (8TMS); 59	Ornithine; Arginine	64	-0.275	-0.291	30.288	0.391	125	17	113	29	137	105 duplicate
13921	135 [902; Melibiose (8TMS); 32	[729; N,N-Dimethyllysine methyl ester]	63	-0.275	-0.427	21.331	0.494	126	16	126	16	108	25 duplicate
15621	135 [902; Melibiose (8TMS); 49	[877; Pyrophosphoric acid (4TMS)]	64	-0.282	-0.452	26.915	0.386	127	15	128	14	133	111 duplicate
11161	135 [902; Melibiose (8TMS); 9	Proline	63	-0.283	-0.349	20.237	0.359	128	14	120	22	101	127 duplicate
13812	135 [902; Melibiose (8TMS); 31	[622; Parabanic acid (2TMS)]	64	-0.287	-0.455	17.387	0.451	129	13	129	13	84	63 duplicate
18564	135 [902; Melibiose (8TMS); 89	[775; Dopamine (4TMS)]	35	-0.291	-0.503	19.917	0.401	130	12	132	10	99	93 duplicate
19835	135 [902; Melibiose (8TMS); 131	[826; 5-Methylthioadenosine (3TMS)]	55	-0.304	-0.515	22.846	0.435	131	11	133	9	116	74 duplicate
10491	135 [902; Melibiose (8TMS); 4	Phosphoric acid	51	-0.315	-0.292	23.664	0.341	132	10	114	28	120	137 duplicate
19825	135 [902; Melibiose (8TMS); 130	Trehalose	63	-0.323	-0.382	19.067	0.430	133	9	123	19	94	76 duplicate
17735	135 [902; Melibiose (8TMS); 75	Lysine	64	-0.324	-0.280	29.016	0.353	134	8	111	31	136	132 duplicate
16477	135 [902; Melibiose (8TMS); 58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64	-0.343	-0.219	8.404	0.360	135	7	103	39	20	125 duplicate
15054	135 [902; Melibiose (8TMS); 43	[548; Leucine (2TMS)]	60	-0.360	-0.483	8.779	0.378	136	6	130	12	24	118 duplicate
18977	135 [902; Melibiose (8TMS); 98	[697; Ribose-5-phosphate methoxamine (5TMS)]	48	-0.369	-0.652	24.793	0.437	137	5	139	3	126	71 duplicate
10216	135 [902; Melibiose (8TMS); 2	Serine	62	-0.375	-0.394	14.529	0.355	138	4	124	18	69	131 duplicate
12904	135 [902; Melibiose (8TMS); 23	Homoserine	64	-0.383	-0.651	12.436	0.489	139	3	137	5	51	28 duplicate
13137	135 [902; Melibiose (8TMS); 25	[709; 2,5-Diaminovalerolactam (2TMS)]	48	-0.429	-0.666	19.652	0.432	140	2	140	2	98	75 duplicate

13366	135 [902; Melibiose (8TMS); 27	1815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	-0.440	-0.695	24,062	0.484	141	1	141	1	122	36 duplicate
17865	136 [748; D-Sedoheptulose-77	benzenesuccinic acid methyl ester]	16	0.667	11,892	0.393	1	139	1	139	106	59 duplicate
15803	136 [748; D-Sedoheptulose-51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	10	0.644	12,347	0.271	2	138	2	138	110	116 duplicate
18170	136 [748; D-Sedoheptulose-82	Lysine	12	0.545	3,218	0.333	3	137	4	136	10	87 duplicate
17325	136 [748; D-Sedoheptulose-69	Arginine	17	0.485	7,112	0.488	4	135	3	137	30	13 duplicate
14957	136 [748; D-Sedoheptulose-42	Glutamic acid	17	0.485	9,928	0.220	5	136	7	133	87	126 duplicate
13922	136 [748; D-Sedoheptulose-32	[729; N,N-Dimethyllysine methyl ester]	17	0.441	0.599	7,288	0.288	6	134	6	134	66
18111	136 [748; D-Sedoheptulose-81	Tyrosine	17	0.412	0.491	13,463	0.321	7	133	18	122	117
19650	136 [748; D-Sedoheptulose-119	[931; myo-Inositol-2-phosphate (7TMS)]	17	0.397	0.463	3,026	0.369	8	131	19	121	8
14452	136 [748; D-Sedoheptulose-37	Phenylalanine	17	0.397	0.472	10,406	0.273	9	132	20	120	83
19728	136 [748; D-Sedoheptulose-123	[945; Galactofuranose-6-phosphate (7TMS)]	17	0.382	0.507	5,522	0.467	10	129	15	125	47
13703	136 [748; D-Sedoheptulose-30	[815; Ethyl-3(2H)-thiophenone]	17	0.382	0.448	12,370	0.317	11	130	23	117	111
16560	136 [748; D-Sedoheptulose-59	Omitidine; Arginine	17	0.368	0.548	19,177	0.291	12	128	10	130	136
9930	136 [748; D-Sedoheptulose-138	[674; Ergosterol (1TMS)]	17	0.353	0.539	7,941	0.349	13	126	11	129	76
14030	136 [748; D-Sedoheptulose-33	Methionine	17	0.353	0.425	4,017	0.194	14	127	27	113	24
19790	136 [748; D-Sedoheptulose-127	[777; Fructose-6-phosphate methoxamine (6TMS)]	17	0.338	0.465	2,882	0.369	15	125	21	119	4
11162	136 [748; D-Sedoheptulose-9	Proline	16	0.333	0.630	11,160	0.377	16	124	5	135	103
10217	136 [748; D-Sedoheptulose-2	Serine	17	0.324	0.554	6,442	0.263	17	122	9	131	57
17180	136 [748; D-Sedoheptulose-67	Citric acid	17	0.324	0.409	11,053	0.283	18	123	31	109	101
19853	136 [748; D-Sedoheptulose-133	[855; Squalene]	17	0.309	0.497	3,635	0.314	19	121	16	124	16
11030	136 [748; D-Sedoheptulose-8	Isoleucine	17	0.294	0.559	6,337	0.187	20	120	8	132	58
16641	136 [748; D-Sedoheptulose-60	Glycerol-3-phosphate	17	0.279	0.457	9,924	0.288	21	118	22	118	86
14137	136 [748; D-Sedoheptulose-141	Lanosta-8,24-dien-3-beta-ol	17	0.279	0.338	14,641	0.172	22	119	42	98	123
9933	136 [748; D-Sedoheptulose-7	Threonine	16	0.267	0.524	5,128	0.376	23	117	13	127	42
19556	136 [748; D-Sedoheptulose-115	Glucose-6-phosphate	17	0.265	0.525	14,552	0.286	24	112	12	128	121
12427	136 [748; D-Sedoheptulose-19	Alanine (BP) (3TMS)	17	0.265	0.437	14,630	0.530	25	113	35	115	122
19320	136 [748; D-Sedoheptulose-107	9-(Z)-Octadecenoic acid	17	0.265	0.385	7,061	0.319	26	114	25	105	64
19446	136 [748; D-Sedoheptulose-111	[583; Erythritol (4TMS)]	17	0.265	0.356	5,960	0.323	27	115	40	100	52
19803	136 [748; D-Sedoheptulose-128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	17	0.265	0.256	11,211	0.316	28	116	55	85	104
19503	136 [748; D-Sedoheptulose-113	Galactose-6-phosphate	17	0.250	0.447	4,744	0.452	29	110	24	116	37
13813	136 [748; D-Sedoheptulose-31	[622; Parabanic acid (2TMS)]	17	0.235	0.424	2,853	0.469	30	111	28	112	3
14858	136 [748; D-Sedoheptulose-41	[639; Proline (2TMS)]	17	0.235	0.395	6,334	0.381	31	108	33	107	55
19776	136 [748; D-Sedoheptulose-126	[559; Erythritol (4TMS)]	17	0.221	0.523	3,476	0.388	32	109	39	101	74
19530	136 [748; D-Sedoheptulose-114	Fructose-6-phosphate	17	0.221	0.382	2,888	0.461	33	104	14	126	14
17466	136 [748; D-Sedoheptulose-71	[731; Erythrose (3TMS)]	17	0.221	0.375	5,630	0.344	34	105	34	108	5
9929	136 [748; D-Sedoheptulose-137	Ergosterol	17	0.221	0.366	7,638	0.356	35	106	38	104	49
19845	136 [748; D-Sedoheptulose-132	[895; Isomaltose methoxamine (8TMS)]	15	0.219	0.420	2,984	0.376	37	103	29	111	6
9931	136 [748; D-Sedoheptulose-139	[700; Ergosta-5,7-dien-3-ol]	14	0.209	0.413	10,681	0.281	38	102	30	110	98
12905	136 [748; D-Sedoheptulose-23	Homoserine	17	0.191	0.283	5,303	0.326	39	101	51	89	45
19475	136 [748; D-Sedoheptulose-112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	17	0.176	0.329	7,654	0.348	40	100	46	94	72
18228	136 [748; D-Sedoheptulose-83	Sorbitol	16	0.167	0.493	10,647	0.226	41	99	17	123	96
16478	136 [748; D-Sedoheptulose-58	(1TMS)]	17	0.132	0.290	6,836	0.265	47	92	50	90	61
19866	136 [748; D-Sedoheptulose-15	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	17	0.162	0.338	5,846	0.400	42	87	43	97	51
11933	136 [748; D-Sedoheptulose-96	myo-Inositol	16	0.150	0.297	8,629	0.391	43	98	49	91	81
18891	136 [748; D-Sedoheptulose-48	Asparagine	17	0.147	0.338	5,263	0.403	45	95	44	96	44
15530	136 [748; D-Sedoheptulose-87	[945; beta-D-Glucopyranose (5TMS)]	16	0.133	0.360	18,498	0.517	46	94	38	102	135
18450	136 [748; D-Sedoheptulose-83	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	17	0.132	0.290	6,836	0.265	47	92	50	90	61

11807	136 [748; D-Sedoheptulose-14	Fumaric acid	17	0.132	0.046	3.651	0.417	48	93	79	61	17	49 duplicate
9832	136 [748; D-Sedoheptulose-140	[692; Ergosta-7,22-dien-3-ol (1TMS)]	14	0.121	0.201	7.454	0.344	49	91	66	74	68	80 original
17670	136 [748; D-Sedoheptulose-74	[912; Tetradecanoic acid (1TMS)]	17	0.118	0.332	3.506	0.329	50	88	45	95	58	90 duplicate
19628	136 [748; D-Sedoheptulose-118	[928; Glucopyranose-6-phosphate (6TMS)]	17	0.118	0.221	3.803	0.319	51	89	63	77	20	95 duplicate
13480	136 [748; D-Sedoheptulose-28	Malic acid	17	0.118	0.027	5.111	0.445	52	90	80	60	41	35 duplicate
15248	136 [748; D-Sedoheptulose-45	Homocysteine	15	0.105	0.279	12.078	0.373	53	87	52	88	108	69 duplicate
18800	136 [748; D-Sedoheptulose-94	Hexadecanoic acid	17	0.103	0.428	14.319	0.354	54	81	26	114	119	74 duplicate
19385	136 [748; D-Sedoheptulose-109	Octadecanoic acid	17	0.103	0.404	17.074	0.414	55	82	32	108	130	53 duplicate
19416	136 [748; D-Sedoheptulose-110	[715; Erythritol (4TMS)]	17	0.103	0.230	4.671	0.474	56	83	59	81	35	19 duplicate
19691	136 [748; D-Sedoheptulose-121	[657; Erythritol (4TMS)]	17	0.103	0.213	4.203	0.421	57	84	64	76	26	47 duplicate
19140	136 [748; D-Sedoheptulose-102	[904; Galactose methoxamine (5TMS)]	17	0.103	0.192	2.986	0.466	58	85	68	72	7	14 duplicate
17990	136 [748; D-Sedoheptulose-79	Glucose	17	0.103	0.092	18.222	0.380	59	86	73	67	134	65 duplicate
19581	136 [748; D-Sedoheptulose-116	[882; Pseudouridine (5TMS)]	13	0.103	0.228	2.463	0.382	60	80	60	80	2	63 duplicate
19605	136 [748; D-Sedoheptulose-117	[724; Glycerol (3TMS)]	17	0.088	0.247	4.617	0.478	61	79	56	84	34	18 duplicate
14243	136 [748; D-Sedoheptulose-35	Pyroglutamic acid	17	0.074	0.341	22.268	0.532	62	77	41	99	139	6 duplicate
	136 [748; D-Sedoheptulose-124	[734; 1-Monodeoxyglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	17	0.074	0.260	11.948	0.457	63	78	54	86	107	30 duplicate
15055	136 [748; D-Sedoheptulose-43	[548; Leucine (2TBS)]	15	0.067	0.244	3.887	0.150	64	76	57	83	23	132 duplicate
17928	136 [748; D-Sedoheptulose-78	Mannose	17	0.059	0.272	3.585	0.484	65	74	53	87	15	15 duplicate
18606	136 [748; D-Sedoheptulose-90	[910; 9-(2)-Hexadecanoic acid (1TMS)]	17	0.059	-0.056	3.475	0.314	66	75	86	54	13	101 duplicate
10355	136 [748; D-Sedoheptulose-3	Ethanolamine	16	0.050	0.222	6.128	0.416	67	73	62	78	54	51 duplicate
18846	136 [748; D-Sedoheptulose-95	[770; 3,4,6-Trisubstitutedphenylmethanolamine (5TMS)]	7	0.048	-0.212	8.087	0.001	68	72	101	39	79	138 duplicate
13253	136 [748; D-Sedoheptulose-28	Citramalic acid	17	0.044	-0.100	8.058	0.417	69	71	87	53	77	50 duplicate
18753	136 [748; D-Sedoheptulose-93	[607; Putrescine (4TMS)]	16	0.033	-0.152	9.329	0.215	70	70	96	44	83	127 duplicate
19353	136 [748; D-Sedoheptulose-108	Octadecanoic acid	17	0.029	0.222	4.614	0.255	71	67	61	79	33	122 duplicate
19061	136 [748; D-Sedoheptulose-100	[857; Mammilol (6TMS)]	17	0.029	0.088	4.841	0.559	72	68	74	66	39	1 duplicate
11293	136 [748; D-Sedoheptulose-10	Glycine	17	0.029	-0.002	5.182	0.456	73	69	83	57	43	31 duplicate
16153	136 [748; D-Sedoheptulose-55	[612; 4-Aminobutyric acid (2TBS)]	11	0.018	0.007	14.337	0.306	74	66	82	58	120	103 duplicate
19710	136 [748; D-Sedoheptulose-122	[644; Erythritol (4TMS)]	17	0.015	0.173	3.665	0.472	75	84	70	70	18	22 duplicate
19178	136 [748; D-Sedoheptulose-103	[648; Ethylamine (2TMS)]	17	0.015	-0.101	9.366	0.261	76	65	88	52	85	121 duplicate
19286	136 [748; D-Sedoheptulose-106	[733; Threitol (4TMS)]	17	0.000	0.060	7.267	0.473	77	61	77	63	65	20 duplicate
18341	136 [748; D-Sedoheptulose-85	[528; Methylcitric acid (4TMS)]	13	0.000	0.019	2.459	0.353	78	62	81	59	1	76 duplicate
18935	136 [748; D-Sedoheptulose-97	[756; beta-D-Methylglucopyranoside (4TMS)]	17	0.000	-0.274	12.612	0.422	79	63	107	33	112	46 duplicate
17736	136 [748; D-Sedoheptulose-75	Lysine	17	-0.015	0.311	19.413	0.321	80	59	48	92	137	94 duplicate
16955	136 [748; D-Sedoheptulose-64	[789; Tyramine (3TMS)]	17	-0.015	0.092	3.112	0.332	81	60	72	68	9	89 duplicate
17603	136 [748; D-Sedoheptulose-73	[708; Glucose methoxamine (5TMS)]	17	-0.015	0.313	3.852	0.472	82	57	47	93	22	21 duplicate
18051	136 [748; D-Sedoheptulose-80	[772; D-Glucose (5TMS)]	16	-0.017	-0.114	15.697	0.462	83	58	90	50	127	28 duplicate
15152	136 [748; D-Sedoheptulose-27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	13	-0.026	0.192	13.381	0.096	84	56	69	71	116	135 duplicate
15622	136 [748; D-Sedoheptulose-44	[910; 2-Ketogluconic acid methoxamine (4TMS)]	17	-0.029	0.074	6.780	0.413	85	53	76	84	60	54 duplicate
18705	136 [748; D-Sedoheptulose-49	[877; Pyrophosphoric acid (4TMS)]	17	-0.029	-0.005	14.693	0.365	86	54	84	56	124	72 duplicate
18705	136 [748; D-Sedoheptulose-92	[680; Glyceral-2-phosphate (4TMS)]	17	-0.029	-0.148	3.757	0.468	87	55	95	45	19	26 duplicate
19215	136 [748; D-Sedoheptulose-104	[795; Erythritol (4TMS)]	17	-0.044	0.052	4.700	0.263	88	52	78	62	36	119 duplicate
12787	136 [748; D-Sedoheptulose-22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	16	-0.050	-0.104	4.155	0.432	89	51	89	51	25	42 duplicate
10628	136 [748; D-Sedoheptulose-5	Leucine	11	-0.055	-0.038	8.245	0.019	90	50	85	55	80	137 duplicate
18978	136 [748; D-Sedoheptulose-98	[697; Ribose-5-phosphate methoxamine (5TMS)]	9	-0.056	-0.186	12.201	0.125	91	48	98	42	109	133 duplicate
15892	136 [748; D-Sedoheptulose-62	[NA]	9	-0.056	-0.391	10.672	0.112	92	49	121	19	97	134 duplicate
17106	136 [748; D-Sedoheptulose-56	Glyceric acid-3-phosphate	17	-0.059	0.203	3.837	0.448	93	46	65	75	21	33 duplicate
12305	136 [748; D-Sedoheptulose-18	[590; 1-Acetyl-2-thiohydantoin]	17	-0.059	-0.120	4.767	0.281	94	47	92	48	38	108 duplicate
19101	136 [748; D-Sedoheptulose-101	[832; Dopamine (4TMS)]	17	-0.074	-0.211	7.478	0.253	95	44	100	40	69	123 duplicate
18656	136 [748; D-Sedoheptulose-91	[766; beta-D-Methylglucopyranoside (4TMS)]	17	-0.074	-0.302	10.744	0.300	96	45	109	31	99	105 duplicate
13138	136 [748; D-Sedoheptulose-25	[709; 2,5-Diaminovalerolactam (2TMS)]	16	-0.083	0.237	10.099	0.415	97	43	58	82	89	52 duplicate

19826	136 [748; D-Sedoheptulose-130	Trehalose	17	-0,088	0,110	13,758	0,307	98	40	71	69	118	102 duplicate
14348	136 [748; D-Sedoheptulose-38	[596; N-Acetylglutamic acid (2TMS)]	17	-0,088	0,078	13,214	0,332	99	41	75	65	114	88 duplicate
16721	136 [748; D-Sedoheptulose-61	[NA]	17	-0,088	-0,283	3,412	0,443	100	42	108	32	12	37 duplicate
19251	136 [748; D-Sedoheptulose-105	[705; 2-Ketogluconic acid (5TMS)]	17	-0,103	-0,174	7,891	0,279	101	38	97	43	75	114 duplicate
16067	136 [748; D-Sedoheptulose-54	[NA]	17	-0,103	-0,386	4,294	0,426	102	39	119	21	28	49 duplicate
19815	136 [748; D-Sedoheptulose-129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc	17	-0,118	-0,354	5,567	0,512	103	37	113	27	48	9 duplicate
18555	136 [748; D-Sedoheptulose-89	[775; Dopamine (4TMS)]	13	-0,128	-0,222	13,133	0,285	104	36	102	38	113	111 duplicate
17801	136 [748; D-Sedoheptulose-76	Fructose	17	-0,132	-0,126	16,099	0,463	105	32	93	47	129	27 duplicate
12668	136 [748; D-Sedoheptulose-21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	17	-0,132	-0,208	8,821	0,334	106	33	99	41	82	85 duplicate
10078	136 [748; D-Sedoheptulose-1	[938; Sulfuric acid (2TMS)]	17	-0,132	-0,342	6,086	0,351	107	34	111	29	53	77 duplicate
15437	136 [748; D-Sedoheptulose-47	[NA]	17	-0,132	-0,373	6,510	0,480	108	35	117	23	59	17 duplicate
11423	136 [748; D-Sedoheptulose-11	Succinic acid	17	-0,147	-0,238	4,265	0,444	109	31	104	36	27	36 duplicate
19860	136 [748; D-Sedoheptulose-134	Isomaltose	17	-0,162	-0,372	16,063	0,506	110	30	116	24	128	10 duplicate
11552	136 [748; D-Sedoheptulose-12	Glyceric acid	17	-0,176	-0,232	6,607	0,409	111	27	103	37	32	56 duplicate
15980	136 [748; D-Sedoheptulose-53	Glycerol-2-phosphate	17	-0,176	-0,253	6,970	0,213	112	28	105	35	63	128 duplicate
17535	136 [748; D-Sedoheptulose-72	[919; D-Xylopyranose (4TMS)]	17	-0,176	-0,260	5,803	0,333	113	29	106	34	50	86 duplicate
18285	136 [748; D-Sedoheptulose-84	Mannitol	16	-0,183	-0,377	15,058	0,303	114	28	118	22	125	104 duplicate
17396	136 [748; D-Sedoheptulose-7	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	16	-0,200	-0,343	11,090	0,418	115	25	112	28	102	48 duplicate
10492	136 [748; D-Sedoheptulose-4	Phosphoric acid	13	-0,205	-0,434	15,246	0,335	116	24	125	15	126	84 duplicate
14758	136 [748; D-Sedoheptulose-40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	17	-0,221	-0,129	17,487	0,354	117	23	94	46	131	75 duplicate
18503	136 [748; D-Sedoheptulose-88	Gluconic acid	17	-0,235	-0,117	6,952	0,431	118	20	91	49	62	43 duplicate
10763	136 [748; D-Sedoheptulose-6	Glycerol	17	-0,235	-0,433	21,255	0,341	119	21	124	16	138	82 duplicate
16395	136 [748; D-Sedoheptulose-57	[757; 2-Desoxy-pentose-3-yose dimethoxyamine (2TMS)]	17	-0,235	-0,458	7,587	0,480	120	22	129	11	70	16 duplicate
18396	136 [748; D-Sedoheptulose-86	[783; D-Galactono-1,4-lactone (4TMS)]	16	-0,250	-0,370	13,330	0,545	121	17	115	25	115	3 duplicate
19020	136 [748; D-Sedoheptulose-99	[682; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	17	-0,250	-0,406	5,062	0,335	122	18	122	18	40	83 duplicate
16800	136 [748; D-Sedoheptulose-62	[812; D-Xylofuranose (4TMS)]	17	-0,250	-0,483	7,451	0,550	123	19	132	8	67	2 duplicate
19761	136 [748; D-Sedoheptulose-125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru	17	-0,265	-0,362	17,710	0,431	124	16	114	26	132	44 duplicate
19671	136 [748; D-Sedoheptulose-120	[945; Uridine (3TMS)]	16	-0,267	-0,524	7,669	0,319	125	15	136	4	73	96 duplicate
15713	136 [748; D-Sedoheptulose-50	[746; Ribonic acid-1,4-lactone (3TMS)]	17	-0,279	-0,421	8,080	0,433	126	14	123	17	78	41 duplicate
14555	136 [748; D-Sedoheptulose-38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	17	-0,284	-0,328	4,606	0,468	127	11	110	30	31	24 duplicate
17031	136 [748; D-Sedoheptulose-65	[846; 3-Deoxyglucitol (5TMS)]	17	-0,294	-0,454	5,371	0,539	128	12	128	12	46	4 duplicate
16311	136 [748; D-Sedoheptulose-56	[829; Orotic acid (3TMS)]	17	-0,294	-0,478	4,514	0,494	129	13	131	9	28	12 duplicate
13592	136 [748; D-Sedoheptulose-29	Erythritol	17	-0,309	-0,442	3,316	0,388	130	8	126	14	11	61 duplicate
11680	136 [748; D-Sedoheptulose-13	Uracil	17	-0,309	-0,449	9,936	0,439	131	9	127	13	88	38 duplicate
15343	136 [748; D-Sedoheptulose-46	Arabinose	17	-0,309	-0,496	10,611	0,537	132	10	133	7	94	5 duplicate
12182	136 [748; D-Sedoheptulose-17	[700; 2-methyl-1,2-propanediol (2TMS)]	17	-0,324	-0,387	10,147	0,436	133	6	120	20	91	40 duplicate
13022	136 [748; D-Sedoheptulose-24	[725; 2-Ketoclanonic acid (2TMS)]	17	-0,324	-0,472	18,183	0,447	134	7	130	10	133	34 duplicate
12058	136 [748; D-Sedoheptulose-16	[644; 2-Methyl-1,3-butanediol (2TMS)]	17	-0,382	-0,503	10,140	0,439	135	5	134	6	90	39 duplicate
19836	136 [748; D-Sedoheptulose-131	[626; 5-Methyladenosine (3TMS)]	12	-0,424	-0,676	11,415	0,281	136	4	138	2	105	112 duplicate
14657	136 [748; D-Sedoheptulose-39	[829; 1-Phenylethanol (1TMS)]	17	-0,441	-0,512	10,645	0,495	137	3	135	5	95	11 duplicate
16878	136 [748; D-Sedoheptulose-63	Glutamine	17	-0,456	-0,605	9,348	0,410	138	2	137	3	84	55 duplicate
12548	136 [748; D-Sedoheptulose-20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	5	-1,000	-0,914	10,881	-0,002	139	1	139	1	100	139 duplicate
17253	136 [748; D-Sedoheptulose-68	[570; Hypoxanthine (2TMS)]	0					140	140	140	140	140	140 duplicate
9937	137 Ergosterol	141 Lanosta-8,24-dien-3-beta-ol	61	0,881	0,983	20,588	0,669	1	141	1	141	93	1 original
9938	137 Ergosterol	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49	0,793	0,947	24,183	0,621	2	140	2	140	113	2 original
9934	137 Ergosterol	138 [674; Ergosterol (1TMS)]	48	0,697	0,698	23,764	0,532	3	139	7	135	111	8 original
19386	137 Ergosterol	109 Octadecanoic acid	64	0,691	0,611	13,042	0,562	4	138	12	130	32	4 duplicate
18801	137 Ergosterol	94 Hexadecanoic acid	84	0,679	0,678	11,686	0,547	5	137	9	133	25	6 duplicate

19582	137 Ergosterol	116 [882; Pseudouridine (5TMS)]	30 0,637	0,789	13,176	0,550	6 136	3 139	34	5 duplicate
19651	137 Ergosterol	119 [931; myo-Inositol-2-phosphate (7TMS)]	64 0,582	0,683	9,434	0,474	7 135	8 134	5	20 duplicate
9935	137 Ergosterol	139 [700; Ergosta-5,7-dien-3-ol (734; 1-Monooctylethanol (1TMS)]	38 0,559	0,738	26,446	0,591	8 134	4 138	128	3 original
19746	137 Ergosterol	124 Monohexadecanoylglycerol (1TMS)]	59 0,516	0,561	31,132	0,419	9 133	14 128	137	48 duplicate
198321	137 Ergosterol	107 9-(2-Octadecenoic acid	64 0,499	0,733	7,564	0,495	10 132	5 137	1	13 duplicate
19854	137 Ergosterol	133 [855; Squalene]	64 0,473	0,715	9,881	0,416	11 131	6 136	6	50 duplicate
19777	137 Ergosterol	126 [559; Erythritol (4TMS)]	45 0,461	0,744	11,685	0,469	12 130	16 126	24	22 duplicate
18342	137 Ergosterol	85 [528; Methylnic acid (4TMS)]	48 0,429	0,615	10,675	0,487	13 129	11 131	15	16 duplicate
16642	137 Ergosterol	60 Glycerol-3-phosphate	64 0,424	0,568	12,701	0,392	14 128	13 129	30	67 duplicate
19354	137 Ergosterol	108 Octadecanoic acid	64 0,405	0,645	13,685	0,388	15 127	10 132	38	70 duplicate
17487	137 Ergosterol	71 [731; Erythrose (3TMS)]	64 0,393	0,330	8,730	0,382	16 128	29 113	3	81 duplicate
17671	137 Ergosterol	74 [912; Tetradecanoic acid (1TMS)]	64 0,389	0,446	14,637	0,412	17 125	18 124	51	52 duplicate
17181	137 Ergosterol	67 Citric acid	64 0,376	0,441	15,400	0,373	18 124	20 122	59	94 duplicate
19447	137 Ergosterol	111 [583; Erythritol (4TMS)]	42 0,361	0,442	25,375	0,386	19 122	19 123	123	73 duplicate
18846	137 Ergosterol	132 [895; Isomaltose methoxamine (8TMS)]	44 0,361	0,118	20,734	0,350	20 123	68 76	94	125 duplicate
15153	137 Ergosterol	44 [910; 2-Ketogluconic acid methoxamine (4TMS)]	50 0,331	0,303	11,455	0,446	21 121	32 110	21	30 duplicate
18607	137 Ergosterol	90 [910; 9-(2-Hexadecenoic acid (1TMS)]	64 0,328	0,499	10,263	0,422	22 120	15 127	10	48 duplicate
18229	137 Ergosterol	83 Sorbitol	58 0,269	0,239	13,786	0,370	23 119	39 103	40	97 duplicate
14453	137 Ergosterol	37 Phenylalanine	64 0,262	0,478	14,291	0,365	24 118	17 125	46	105 duplicate
19711	137 Ergosterol	122 [844; Erythritol (4TMS)]	52 0,261	0,204	21,043	0,415	25 117	48 94	97	51 duplicate
10366	137 Ergosterol	3 Ethanolamine	62 0,243	0,388	17,637	0,373	26 116	24 118	68	92 duplicate
19872	137 Ergosterol	136 [748; D-Sedoheptulose-7-phosphate (7TMS)]	17 0,221	0,366	7,638	0,356	27 115	28 116	2	118 duplicate
18112	137 Ergosterol	81 Tyrosine	64 0,212	0,418	24,323	0,411	28 114	22 120	114	53 duplicate
15893	137 Ergosterol	52 [NA]	46 0,212	0,268	24,171	0,361	29 113	36 106	112	113 duplicate
12549	137 Ergosterol	20 [619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	31 0,209	0,254	20,335	0,530	30 112	37 105	91	9 duplicate
19141	137 Ergosterol	102 [904; Galactose methoxamine (5TMS)]	64 0,193	0,153	14,784	0,365	31 111	53 89	54	104 duplicate
19867	137 Ergosterol	135 [902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	64 0,192	0,208	9,023	0,386	32 110	45 97	4	74 duplicate
14958	137 Ergosterol	42 Glutamic acid	60 0,186	0,373	21,388	0,369	33 109	25 117	102	100 duplicate
17866	137 Ergosterol	[826; beta-[[[5-methyl-2-thienyl)methyl]eneamino- benzeneacetic acid methyl ester]	62 0,186	0,297	21,315	0,350	34 108	33 109	100	126 duplicate
19082	137 Ergosterol	100 [857; Mannitol (6TMS)]	64 0,184	0,079	10,385	0,361	35 107	71 71	11	114 duplicate
19417	137 Ergosterol	110 [715; Erythritol (4TMS)]	54 0,178	0,109	17,691	0,511	36 106	67 75	69	11 duplicate
19476	137 Ergosterol	112 [877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	63 0,177	0,177	24,870	0,360	37 105	49 93	119	115 duplicate
17254	137 Ergosterol	68 [570; Hypoxanthine (2TMS)]	20 0,168	0,282	19,966	0,368	38 104	34 108	87	101 duplicate
18847	137 Ergosterol	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	50 0,164	0,129	24,954	0,365	39 103	61 81	120	106 duplicate
12308	137 Ergosterol	18 [590; 1-Acetyl-2-thiohydantoin]	64 0,162	0,244	10,544	0,402	40 102	38 104	13	56 duplicate
10898	137 Ergosterol	7 Threonine	64 0,161	0,407	21,080	0,381	41 101	23 119	98	82 duplicate
14349	137 Ergosterol	38 [596; N-Acetylglutamic acid (2TMS)]	64 0,159	0,315	19,687	0,379	42 100	31 111	85	85 duplicate
19531	137 Ergosterol	114 Fructose-6-phosphate	53 0,135	0,031	16,600	0,351	43 99	77 65	61	123 duplicate
19608	137 Ergosterol	117 [724; Glycerol (3TMS)]	56 0,122	0,135	14,774	0,394	44 98	59 83	52	65 duplicate
16154	137 Ergosterol	55 [612; 4-Aminobutyric acid (2TMS)]	43 0,118	0,350	28,097	0,433	45 97	28 114	132	36 duplicate
18692	137 Ergosterol	121 [657; Erythritol (4TMS)]	55 0,116	0,145	20,914	0,402	46 96	56 86	96	57 duplicate
19791	137 Ergosterol	127 [777; Fructose-6-phosphate methoxamine (6TMS)]	39 0,112	0,053	11,061	0,377	47 95	73 69	17	84 duplicate
19837	137 Ergosterol	131 [626; 5-Methylthioadenosine (3TMS)]	55 0,108	-0,002	23,487	0,441	48 94	84 58	109	37 duplicate
14759	137 Ergosterol	40 [680; 2,3-Dimethylsuccinic acid (2TMS)]	64 0,107	0,147	25,537	0,433	49 93	55 87	125	37 duplicate
19557	137 Ergosterol	115 Glucose-6-phosphate	62 0,105	-0,090	18,072	0,439	50 92	93 49	74	35 duplicate
12788	137 Ergosterol	22 [690; N,N-Di(2-Hydroxyethyl)-methanamine (2TMS)]	52 0,100	0,097	18,951	0,401	51 91	69 73	79	58 duplicate
13481	137 Ergosterol	28 Malic acid	64 0,097	0,043	10,185	0,442	52 90	75 67	8	32 duplicate

16561	137 Ergosterol	59 Ornithine; Arginine	64 0.090	0.209	31,609	0.355	53	89	44	98	138	119 duplicate
13254	137 Ergosterol	26 Citramalic acid	64 0.077	0.131	10,428	0.370	55	87	80	82	12	89 duplicate
18892	137 Ergosterol	96 myo-Inositol	49 0.075	0.010	27,459	0.363	56	86	80	62	131	108 duplicate
19504	137 Ergosterol	113 Galactose-6-phosphate	62 0.075	-0.105	17,288	0.346	57	85	97	45	66	129 duplicate
11294	137 Ergosterol	10 Glycine	64 0.072	0.168	12,798	0.470	58	84	50	92	31	21 duplicate
15804	137 Ergosterol	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	44 0.070	0.235	25,969	0.365	59	83	41	101	127	76 duplicate
19216	137 Ergosterol	104 [795; Erythritol (4TMS)]	63 0.068	0.079	13,670	0.394	60	82	70	72	37	66 duplicate
19804	137 Ergosterol	128 [824; D-Sedoheptulose-7-phosphate (7TMS)]	45 0.065	-0.031	11,645	0.376	61	81	89	53	23	89 duplicate
16722	137 Ergosterol	61 [NA]	64 0.064	0.151	12,503	0.331	62	80	54	88	29	138 duplicate
17326	137 Ergosterol	19 Arginine	60 0.064	0.120	14,891	0.443	63	79	65	77	58	31 duplicate
11553	137 Ergosterol	12 Glycic acid	63 0.064	0.003	19,631	0.375	64	78	83	59	84	91 duplicate
11808	137 Ergosterol	14 Fumaric acid	64 0.063	0.008	17,806	0.368	65	77	81	61	71	62 duplicate
14859	137 Ergosterol	41 [639; Proline (2TMS)]	64 0.062	0.102	10,161	0.382	66	76	68	74	7	80 duplicate
12428	137 Ergosterol	19 Alanine (BP) (3TMS)	64 0.053	0.043	11,091	0.425	67	75	74	68	19	59 duplicate
12669	137 Ergosterol	21 [678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	64 0.051	0.060	11,079	0.425	68	74	72	70	18	44 duplicate
18827	137 Ergosterol	130 Trehalose	63 0.037	0.204	21,343	0.338	69	73	47	95	101	138 duplicate
13704	137 Ergosterol	30 [815; Ethyl-3-(2H)-thiophenone]	64 0.037	0.137	21,765	0.372	70	72	58	84	106	85 duplicate
14244	137 Ergosterol	35 Pyroglutamic acid	64 0.036	-0.168	32,583	0.430	71	71	111	31	139	40 duplicate
17802	137 Ergosterol	76 Fructose	64 0.034	-0.133	20,144	0.442	72	70	102	40	88	33 duplicate
15531	137 Ergosterol	48 Asparagine	64 0.031	0.143	14,784	0.419	73	69	57	85	53	47 duplicate
19672	137 Ergosterol	120 [945; Uridine (3TMS)]	54 0.027	-0.105	10,658	0.367	74	68	86	46	14	102 duplicate
17829	137 Ergosterol	78 Mannose	62 0.023	-0.009	18,918	0.486	75	67	86	56	78	17 duplicate
19287	137 Ergosterol	108 [733; Threitol (4TMS)]	62 0.021	-0.024	14,847	0.493	76	68	88	54	55	15 duplicate
13923	137 Ergosterol	32 [729; N,N-Dimethyllysine methyl ester]	63 0.016	0.223	21,170	0.397	77	65	43	89	99	63 duplicate
17737	137 Ergosterol	75 Lysine	64 0.011	0.279	30,280	0.362	78	64	35	107	136	110 duplicate
14031	137 Ergosterol	53 Methionine	64 0.005	0.122	14,014	0.399	79	63	84	78	43	60 duplicate
15981	137 Ergosterol	53 Glycerol-2-phosphate	64 -0.003	-0.031	19,470	0.343	80	62	90	52	82	131 duplicate
16879	137 Ergosterol	63 Glutamine	52 -0.011	0.205	20,157	0.385	81	61	46	96	88	75 duplicate
11163	137 Ergosterol	9 Proline	63 -0.011	0.323	19,122	0.381	82	60	30	112	80	83 duplicate
13814	137 Ergosterol	31 [622; Parabanic acid (2TMS)]	64 -0.013	0.162	18,602	0.361	83	58	51	91	77	112 duplicate
19729	137 Ergosterol	123 [945; Galactofuranose-6-phosphate (7TMS)]	64 -0.013	-0.005	10,210	0.387	84	59	85	57	9	71 duplicate
18286	137 Ergosterol	84 Mannitol	62 -0.015	-0.310	25,759	0.342	85	57	132	10	126	132 duplicate
11031	137 Ergosterol	8 Isoleucine	55 -0.021	0.438	11,998	0.380	86	56	21	121	26	84 duplicate
14138	137 Ergosterol	34 Aspartic acid	64 -0.022	0.032	24,372	0.384	87	55	76	66	115	77 duplicate
19252	137 Ergosterol	105 [705; 2-Ketogluconic acid (5TMS)]	48 -0.023	-0.157	15,025	0.417	88	54	107	35	57	49 duplicate
18706	137 Ergosterol	92 [880; Glycerol-2-phosphate (4TMS)]	54 -0.023	-0.246	15,815	0.376	89	53	124	18	60	90 duplicate
17604	137 Ergosterol	73 [708; Glucose methoxamine (5TMS)]	57 -0.025	0.023	17,800	0.429	90	52	78	64	70	41 duplicate
17107	137 Ergosterol	66 Glycic acid-3-phosphate	64 -0.033	0.228	14,512	0.395	91	51	42	100	48	64 duplicate
16068	137 Ergosterol	54 [NA]	55 -0.036	-0.161	19,869	0.348	92	50	109	33	86	128 duplicate
16479	137 Ergosterol	[636; 4R-Acetylido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	64 -0.040	0.159	11,350	0.353	93	49	52	90	20	121 duplicate
16396	137 Ergosterol	57 [757; 2-Desoxy-pentose-3-yose dimethoxamine (2TMS)]	55 -0.040	-0.089	17,076	0.431	94	48	92	50	65	39 duplicate
10493	137 Ergosterol	4 Phosphoric acid	51 -0.040	0.236	23,428	0.405	95	47	40	102	108	55 duplicate
15714	137 Ergosterol	120 [746; Ribonic acid-1,4-lactone (3TMS)]	61 -0.042	-0.127	26,726	0.370	96	46	100	42	129	98 duplicate
19762	137 Ergosterol	125 [892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	64 -0.051	-0.260	25,505	0.371	97	45	128	14	124	96 duplicate
10218	137 Ergosterol	2 Serine	62 -0.054	0.356	13,759	0.359	98	44	27	115	39	117 duplicate
17536	137 Ergosterol	72 [919; D-Xylopyranose (4TMS)]	63 -0.055	-0.193	17,419	0.331	99	43	117	25	87	137 duplicate
11424	137 Ergosterol	11 Succinic acid	64 -0.056	-0.094	11,554	0.351	100	42	85	47	22	122 duplicate
14566	137 Ergosterol	38 [708; 2,3-Dimethylsuccinic acid (2TMS)]	64 -0.057	-0.092	12,179	0.427	101	41	94	48	27	43 duplicate
18801	137 Ergosterol	62 [812; D-Xylofuranose (4TMS)]	64 -0.064	-0.203	10,891	0.432	102	40	119	23	16	38 duplicate

18754	137 Ergosterol	93 [607; Putrescine (4TMS)]	60 -0.070	-0.276	25.091	0.363	103	39	129	13	121	79 duplicate
18171	137 Ergosterol	82 Lysine	39 -0.072	-0.134	13.167	0.544	104	36	104	38	33	7 duplicate
15623	137 Ergosterol	49 [877; Pyrophosphoric acid (4TMS)]	64 -0.073	-0.132	28.206	0.351	105	37	101	41	133	124 duplicate
17397	137 Ergosterol	70 [693; 2-Furan-2-hydroxyacetic acid (2TMS)]	57 -0.076	-0.258	14.242	0.373	106	36	127	15	44	93 duplicate
18397	137 Ergosterol	86 [793; D-Galactono-1,4-lactone (4TMS)]	61 -0.080	-0.186	22.067	0.518	107	35	116	26	107	10 duplicate
19629	137 Ergosterol	118 [928; Glucopyranose-6-phosphate (6TMS)]	58 -0.088	-0.257	16.874	0.336	108	34	128	16	63	135 duplicate
10829	137 Ergosterol	5 Leucine	45 -0.091	-0.322	16.981	0.447	109	33	133	8	64	29 duplicate
18979	137 Ergosterol	98 [697; Ribose-5-phosphate methoxymine (5TMS)]	48 -0.110	0.126	24.515	0.327	110	32	62	80	117	140 duplicate
18504	137 Ergosterol	88 Gluconic acid	64 -0.112	-0.064	13.987	0.454	111	31	91	51	42	28 duplicate
18916	137 Ergosterol	[940; Maltose methoxymine (8TMS); alpha-D-Glc-(1,4)-D-129 Glc]	59 -0.121	-0.133	17.855	0.459	112	30	103	39	72	26 duplicate
18556	137 Ergosterol	89 [775; Dopamine (4TMS)]	35 -0.126	0.123	20.899	0.383	113	29	63	79	95	78 duplicate
13593	137 Ergosterol	29 Erythritol	64 -0.128	-0.152	13.825	0.406	114	28	105	37	41	54 duplicate
14658	137 Ergosterol	39 [829; 1-Phenylethanol (1TMS)]	63 -0.137	-0.114	16.668	0.427	115	27	98	44	62	42 duplicate
15344	137 Ergosterol	46 Arabinose	64 -0.140	-0.222	19.618	0.468	116	26	122	20	83	23 duplicate
15249	137 Ergosterol	45 Homocysteine	61 -0.142	-0.162	29.528	0.353	117	25	110	32	135	120 duplicate
17032	137 Ergosterol	65 [646; 3-Deoxyglucitol (5TMS)]	63 -0.154	-0.179	21.541	0.467	118	24	113	29	105	24 duplicate
11681	137 Ergosterol	13 Uracil	64 -0.155	-0.170	14.267	0.480	119	23	112	30	45	18 duplicate
10764	137 Ergosterol	6 Glycerol	64 -0.158	-0.254	33.058	0.364	120	22	125	17	140	107 duplicate
18861	137 Ergosterol	134 Isomaltose	64 -0.159	-0.200	21.518	0.493	121	21	118	24	104	14 duplicate
12906	137 Ergosterol	23 Homoserine	64 -0.167	0.004	14.516	0.390	122	19	82	60	49	68 duplicate
13023	137 Ergosterol	24 [725; 2-Ketocotanoic acid (2TMS)]	64 -0.167	-0.180	24.588	0.499	123	20	114	28	118	12 duplicate
16312	137 Ergosterol	56 [829; Orotic acid (3TMS)]	64 -0.176	-0.235	20.185	0.467	124	18	123	19	90	25 duplicate
12059	137 Ergosterol	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	64 -0.177	-0.183	13.553	0.480	125	17	115	27	35	19 duplicate
18656	137 Ergosterol	84 [789; Tyramine (3TMS)]	63 -0.190	-0.127	13.639	0.399	126	16	89	43	38	61 duplicate
18451	137 Ergosterol	87 [945; beta-D-Glucopyranose (5TMS)]	62 -0.193	-0.281	28.626	0.338	127	15	131	11	134	133 duplicate
17991	137 Ergosterol	79 Glucose	64 -0.210	-0.212	27.196	0.367	128	14	121	21	130	103 duplicate
18936	137 Ergosterol	97 [756; beta-D-Methylglucopyranoside (4TMS)]	52 -0.210	-0.380	21.499	0.325	129	13	138	4	103	141 duplicate
13368	137 Ergosterol	27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	53 -0.210	0.018	24.512	0.367	130	12	79	63	116	72 duplicate
19179	137 Ergosterol	103 [648; Ethylamine (2TMS)]	63 -0.221	-0.357	19.327	0.362	131	11	135	7	81	111 duplicate
12183	137 Ergosterol	17 [700; 2-methyl-1,2-propanediol (2TMS)]	64 -0.221	-0.205	14.323	0.363	132	10	120	22	47	109 duplicate
19021	137 Ergosterol	99 [662; Ribose-5-phosphate methoxymine (BP) (5TMS)]	41 -0.239	-0.161	17.897	0.377	133	9	108	34	73	88 duplicate
11934	137 Ergosterol	15 Alanine	64 -0.250	-0.281	14.568	0.454	134	8	130	12	50	27 duplicate
15056	137 Ergosterol	43 [548; Leucine (2TBS)]	60 -0.258	-0.342	12.286	0.388	135	7	134	8	28	69 duplicate
18052	137 Ergosterol	80 [772; D-Glucose (5TMS)]	62 -0.266	-0.367	25.255	0.328	136	6	137	5	122	139 duplicate
13139	137 Ergosterol	25 [709; 2,5-Diaminovalerolactam (2TMS)]	48 -0.282	-0.156	20.436	0.423	137	5	108	36	92	45 duplicate
18657	137 Ergosterol	91 [766; beta-D-Methylglucopyranoside (4TMS)]	64 -0.315	-0.493	23.488	0.349	138	4	140	2	110	127 duplicate
10079	137 Ergosterol	1 [938; Sulfuric acid (2TMS)]	36 -0.317	-0.363	15.141	0.337	139	3	136	6	58	134 duplicate
15438	137 Ergosterol	47 [NA]	64 -0.334	-0.438	18.188	0.360	140	2	139	3	76	116 duplicate
19102	137 Ergosterol	101 [832; Dopamine (4TMS)]	64 -0.335	-0.521	18.083	0.379	141	1	141	1	75	88 duplicate
9940	138 [674; Ergosterol (1TMS)]	141 Lanosta-8,24-dien-3-beta-ol	45 0.731	0.867	6.570	0.644	1	140	2	139	8	1 original
19387	138 [674; Ergosterol (1TMS)]	109 Octadecanoic acid	46 0.697	0.818	31.639	0.496	2	138	4	137	115	15 duplicate
19877	138 [674; Ergosterol (1TMS)]	137 Ergosterol	46 0.697	0.698	23.764	0.532	3	139	8	133	94	8 duplicate
19583	138 [674; Ergosterol (1TMS)]	116 [882; Pseudouridine (5TMS)]	27 0.687	0.682	8.365	0.472	4	137	10	131	13	32 duplicate
18802	138 [674; Ergosterol (1TMS)]	94 Hexadecanoic acid	46 0.693	0.882	31.071	0.585	5	138	1	140	113	5 duplicate
9939	138 [674; Ergosterol (1TMS)]	140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	43 0.661	0.810	2.687	0.601	6	135	5	138	1	3 original
19855	138 [674; Ergosterol (1TMS)]	133 [855; Squalene]	48 0.627	0.832	15.921	0.606	7	134	3	138	81	2 duplicate
18343	138 [674; Ergosterol (1TMS)]	85 [529; Methylcitric acid (4TMS)]	34 0.601	0.755	10.727	0.534	8	133	6	135	31	7 duplicate
17672	138 [674; Ergosterol (1TMS)]	74 [912; Tetradecanoic acid (1TMS)]	46 0.498	0.741	14.981	0.486	9	132	7	134	56	16 duplicate
19747	138 [674; Ergosterol (1TMS)]	124 Monohexadecanoylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	46 0.459	0.590	6.255	0.484	10	131	11	130	6	23 duplicate



19532	138 [674; Ergosterol (1TMS) 114	Fructose-6-phosphate	41	0.439	0.543	10.107	0.505	11	129	16	125	22	14 duplicate
18230	138 [674; Ergosterol (1TMS) 83	Sorbitol	41	0.439	0.395	27.648	0.372	12	130	30	111	109	112 duplicate
19448	138 [674; Ergosterol (1TMS) 111	[583; Erythritol (4TMS)]	32	0.435	0.549	5.643	0.469	13	128	14	127	4	35 duplicate
17468	138 [674; Ergosterol (1TMS) 71	[731; Erythrose (3TMS)]	46	0.432	0.580	21.698	0.445	14	127	13	128	86	52 duplicate
19778	138 [674; Ergosterol (1TMS) 126	[559; Erythritol (4TMS)]	32	0.419	0.687	11.949	0.441	15	126	9	132	36	53 duplicate
19847	138 [674; Ergosterol (1TMS) 132	[895; Isomaltose methoxyamine (8TMS)]	33	0.394	0.377	10.337	0.376	16	125	34	107	26	106 duplicate
16843	138 [674; Ergosterol (1TMS) 60	Glycerol-3-phosphate	46	0.387	0.585	30.129	0.451	17	124	12	129	112	47 duplicate
19505	138 [674; Ergosterol (1TMS) 113	Galactose-6-phosphate	45	0.358	0.325	12.080	0.426	18	123	41	100	39	68 duplicate
19873	138 [674; Ergosterol (1TMS) 136	[748; D-Scdheptulose-7-phosphate (7TMS)]	17	0.353	0.539	7.941	0.349	19	122	17	124	11	126 duplicate
19558	138 [674; Ergosterol (1TMS) 115	Glucose-6-phosphate	45	0.345	0.305	32.658	0.411	20	121	44	97	117	77 duplicate
19730	138 [674; Ergosterol (1TMS) 123	[945; Galactofuranose-6-phosphate (7TMS)]	46	0.333	0.539	19.487	0.535	21	120	18	123	80	6 duplicate
19652	138 [674; Ergosterol (1TMS) 119	[931; myo-Inositol-2-phosphate (7TMS)]	46	0.329	0.490	17.662	0.481	22	119	19	122	69	25 duplicate
9938	138 [674; Ergosterol (1TMS) 139	[700; Ergosta-5,7-dien-3-ol]	36	0.317	0.486	5.789	0.403	23	118	20	121	5	84 original
12429	138 [674; Ergosterol (1TMS) 19	Alanine (BP) (3TMS)	46	0.308	0.477	20.632	0.473	24	117	21	120	82	31 duplicate
14860	138 [674; Ergosterol (1TMS) 41	[639; Proline (2TMS)]	46	0.302	0.543	22.688	0.435	25	116	15	126	90	60 duplicate
19712	138 [674; Ergosterol (1TMS) 122	[644; Erythritol (4TMS)]	36	0.273	0.402	10.111	0.471	26	115	28	113	23	34 duplicate
15154	138 [674; Ergosterol (1TMS) 44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	34	0.273	0.362	17.688	0.447	27	114	37	104	70	48 duplicate
17182	138 [674; Ergosterol (1TMS) 67	Citric acid	46	0.270	0.404	32.218	0.377	28	113	27	114	116	104 duplicate
19063	138 [674; Ergosterol (1TMS) 100	[857; Mannitol (6TMS)]	46	0.266	0.282	18.969	0.457	29	112	47	94	76	42 duplicate
19142	138 [674; Ergosterol (1TMS) 102	[904; Galactose methoxyamine (5TMS)]	46	0.264	0.305	12.589	0.469	30	111	45	86	40	36 duplicate
12307	138 [674; Ergosterol (1TMS) 18	[590; 1-Acetyl-2-thiohydantoin]	46	0.262	0.424	17.254	0.364	31	110	24	117	67	119 duplicate
19418	138 [674; Ergosterol (1TMS) 110	[715; Erythritol (4TMS)]	38	0.255	0.342	14.320	0.478	32	109	39	102	51	27 duplicate
14350	138 [674; Ergosterol (1TMS) 36	[596; N-Acetylglutamic acid (2TMS)]	46	0.248	0.474	35.548	0.379	33	108	22	119	122	103 duplicate
18693	138 [674; Ergosterol (1TMS) 121	[657; Erythritol (4TMS)]	38	0.243	0.400	8.053	0.400	34	107	29	112	12	85 duplicate
19217	138 [674; Ergosterol (1TMS) 104	[795; Erythritol (4TMS)]	45	0.240	0.375	14.967	0.397	35	106	35	106	55	88 duplicate
10899	138 [674; Ergosterol (1TMS) 7	Threonine	46	0.229	0.385	37.506	0.365	36	105	32	109	128	117 duplicate
	138 [674; Ergosterol (1TMS) 58	[636; 4R-Acetaldo-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	46	0.227	0.271	23.813	0.392	37	104	49	92	95	94 duplicate
16480	138 [674; Ergosterol (1TMS) 112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	46	0.223	0.374	4.793	0.438	38	103	36	105	2	55 duplicate
19477	138 [674; Ergosterol (1TMS) 28	Malic acid	46	0.219	0.269	19.308	0.422	39	102	50	91	78	69 duplicate
13482	138 [674; Ergosterol (1TMS) 117	[724; Glycerol (3TMS)]	41	0.217	0.408	14.441	0.437	40	101	28	115	53	58 duplicate
18608	138 [674; Ergosterol (1TMS) 135	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	46	0.215	0.453	22.024	0.480	41	100	23	118	87	26 duplicate
14245	138 [674; Ergosterol (1TMS) 35	Pyroglutamic acid	46	0.210	0.165	47.244	0.488	42	99	70	71	140	21 duplicate
17738	138 [674; Ergosterol (1TMS) 75	Lysine	46	0.208	0.337	45.125	0.360	43	97	40	101	137	121 duplicate
14760	138 [674; Ergosterol (1TMS) 40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	46	0.208	0.320	41.586	0.387	44	98	42	99	136	98 duplicate
14454	138 [674; Ergosterol (1TMS) 37	Phenylalanine	46	0.200	0.391	31.191	0.408	45	96	31	110	114	80 duplicate
19828	138 [674; Ergosterol (1TMS) 130	Trehalose	45	0.198	0.264	36.892	0.394	46	95	52	89	127	90 duplicate
12789	138 [674; Ergosterol (1TMS) 22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	37	0.192	0.247	8.546	0.408	47	94	58	83	16	81 duplicate
17803	138 [674; Ergosterol (1TMS) 76	Fructose	46	0.181	0.178	33.690	0.481	48	93	67	74	119	24 duplicate
17630	138 [674; Ergosterol (1TMS) 28	Mannose	46	0.179	0.269	14.061	0.477	49	92	51	90	50	29 duplicate
13255	138 [674; Ergosterol (1TMS) 26	Citramalic acid	46	0.173	0.280	25.775	0.405	50	91	48	93	100	83 duplicate
18893	138 [674; Ergosterol (1TMS) 96	myo-Inositol	39	0.171	0.419	5.491	0.332	51	90	25	116	3	130 duplicate
18113	138 [674; Ergosterol (1TMS) 81	Tyrosine	46	0.161	0.262	40.524	0.476	52	89	53	88	135	30 duplicate
19288	138 [674; Ergosterol (1TMS) 106	[733; Threitol (4TMS)]	46	0.157	0.258	19.404	0.490	53	88	57	84	79	18 duplicate
10357	138 [674; Ergosterol (1TMS) 3	Ethanolamine	44	0.154	0.209	10.393	0.416	54	87	63	78	28	75 duplicate
12670	138 [674; Ergosterol (1TMS) 21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	46	0.150	0.261	25.993	0.337	55	86	54	87	102	129 duplicate
18630	138 [674; Ergosterol (1TMS) 118	[928; Glucopyranose-6-phosphate (6TMS)]	42	0.145	0.207	11.793	0.408	56	85	64	77	34	82 duplicate
11809	138 [674; Ergosterol (1TMS) 14	Fumaric acid	46	0.142	0.206	10.248	0.383	57	84	65	76	25	100 duplicate
17398	138 [674; Ergosterol (1TMS) 70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	43	0.141	0.170	26.974	0.305	58	83	68	73	104	138 duplicate
17892	138 [674; Ergosterol (1TMS) 79	Glucose	46	0.138	0.193	40.209	0.356	59	82	66	75	134	124 duplicate

19322	138 [674; Ergosterol (1TMS)]	107	9-(Z)-Octadecenoic acid	46	0.130	0.315	24.497	0.344	60	81	43	98	97	128 duplicate
19957	138 [674; Ergosterol (1TMS)]	64	[789; Tyramine (3TMS)]	45	0.127	0.237	12.875	0.375	61	80	61	80	44	109 duplicate
14959	138 [674; Ergosterol (1TMS)]	42	Glutamic acid	42	0.106	0.215	34.115	0.306	62	79	62	79	121	135 duplicate
17605	138 [674; Ergosterol (1TMS)]	73	[708; Glucose methoxyamine (5TMS)]	42	0.089	0.291	13.871	0.426	63	78	48	95	49	87 duplicate
18848	138 [674; Ergosterol (1TMS)]	95	[770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	33	0.091	0.096	7.009	0.375	64	77	76	65	10	108 duplicate
	138 [674; Ergosterol (1TMS)]		[826; beta-[(5-methyl-2-thienyl)methylethanol]-											
17887		77	benzeneacetic acid methyl ester]	44	0.089	0.238	35.783	0.355	65	76	60	81	123	125 duplicate
19763	138 [674; Ergosterol (1TMS)]	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	46	0.088	0.087	38.273	0.429	66	75	77	64	129	64 duplicate
10219	138 [674; Ergosterol (1TMS)]	2	Serine	44	0.085	0.382	24.291	0.364	67	74	38	103	96	118 duplicate
16562	138 [674; Ergosterol (1TMS)]	59	Ornithine; Arginine	46	0.067	0.111	46.336	0.319	68	73	73	68	138	133 duplicate
17922	138 [674; Ergosterol (1TMS)]	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	30	0.057	0.100	12.700	0.368	69	72	74	67	41	114 duplicate
11835	138 [674; Ergosterol (1TMS)]	15	Alanine	46	0.053	0.117	25.418	0.388	70	71	72	69	98	97 duplicate
19355	138 [674; Ergosterol (1TMS)]	108	Octadecenoic acid	46	0.049	0.241	12.738	0.421	71	70	59	82	42	70 duplicate
17327	138 [674; Ergosterol (1TMS)]	69	Arginine	43	0.037	0.048	27.267	0.435	72	69	83	58	106	61 duplicate
19673	138 [674; Ergosterol (1TMS)]	120	[945; Uridine (3TMS)]	39	0.036	-0.122	21.158	0.363	73	68	110	31	83	120 duplicate
11534	138 [674; Ergosterol (1TMS)]	12	Glycine acid	45	0.030	0.068	9.026	0.430	74	67	79	62	19	63 duplicate
11164	138 [674; Ergosterol (1TMS)]	9	Proline	45	0.028	0.261	32.818	0.374	75	66	55	88	118	110 duplicate
14557	138 [674; Ergosterol (1TMS)]	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	46	0.014	0.084	17.756	0.430	76	65	78	63	72	62 duplicate
10765	138 [674; Ergosterol (1TMS)]	6	Glycerol	46	-0.001	0.012	47.226	0.357	77	64	93	48	139	122 duplicate
11425	138 [674; Ergosterol (1TMS)]	11	Succinic acid	46	-0.005	0.055	17.870	0.377	78	63	82	59	71	105 duplicate
13924	138 [674; Ergosterol (1TMS)]	32	[729; N,N-Dimethyllysine methyl ester]	45	-0.006	0.169	12.791	0.417	79	82	69	72	43	73 duplicate
16802	138 [674; Ergosterol (1TMS)]	62	[812; D-Xylofuranose (4TMS)]	46	-0.007	0.056	23.705	0.409	80	61	81	60	92	79 duplicate
10494	138 [674; Ergosterol (1TMS)]	4	Phosphoric acid	35	-0.008	0.133	36.553	0.393	81	60	71	70	126	93 duplicate
18608	138 [674; Ergosterol (1TMS)]	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	46	-0.011	0.039	17.244	0.349	82	59	91	60	66	127 duplicate
17108	138 [674; Ergosterol (1TMS)]	68	Glyceric acid-3-phosphate	46	-0.016	0.258	12.029	0.488	83	58	58	85	37	19 duplicate
13705	138 [674; Ergosterol (1TMS)]	30	[815; Ethyl-3(2H)-thiophenone]	46	-0.020	0.047	36.076	0.299	84	57	84	57	124	138 duplicate
18398	138 [674; Ergosterol (1TMS)]	86	[793; D-Galactono-1,4-lactone (4TMS)]	44	-0.025	0.097	29.031	0.511	85	56	75	68	111	13 duplicate
13815	138 [674; Ergosterol (1TMS)]	31	[822; Parabenic acid (2TMS)]	46	-0.032	0.042	9.561	0.382	86	55	86	55	21	101 duplicate
11295	138 [674; Ergosterol (1TMS)]	15	Glycine	46	-0.036	-0.099	27.177	0.452	87	54	107	34	105	45 duplicate
18452	138 [674; Ergosterol (1TMS)]	87	[945; beta-D-Glucopyranose (5TMS)]	44	-0.049	-0.072	40.125	0.398	88	53	80	61	133	89 duplicate
19805	138 [674; Ergosterol (1TMS)]	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	31	-0.049	-0.072	16.886	0.386	89	52	104	37	62	99 duplicate
14032	138 [674; Ergosterol (1TMS)]	33	Methionine	46	-0.055	0.006	17.184	0.304	90	51	96	45	65	137 duplicate
18505	138 [674; Ergosterol (1TMS)]	88	Gluconic acid	46	-0.067	0.040	21.305	0.436	91	50	89	52	84	59 duplicate
18053	138 [674; Ergosterol (1TMS)]	80	[772; D-Glucose (5TMS)]	44	-0.074	0.002	36.104	0.372	92	49	97	44	125	111 duplicate
15715	138 [674; Ergosterol (1TMS)]	50	[746; Ribonic acid-1,4-lactone (3TMS)]	43	-0.083	0.006	6.777	0.438	93	48	95	46	9	57 duplicate
15805	138 [674; Ergosterol (1TMS)]	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	39	-0.083	-0.127	8.765	0.393	94	47	111	30	17	92 duplicate
11032	138 [674; Ergosterol (1TMS)]	8	Isoleucine	46	-0.100	0.383	23.734	0.389	95	46	33	108	93	98 duplicate
16723	138 [674; Ergosterol (1TMS)]	61	[NA]	48	-0.100	-0.159	15.147	0.387	96	45	112	29	57	115 duplicate
14139	138 [674; Ergosterol (1TMS)]	34	Aspartic acid	46	-0.103	-0.096	39.333	0.281	97	44	106	35	130	139 duplicate
15532	138 [674; Ergosterol (1TMS)]	48	Asparagine	46	-0.109	-0.177	18.309	0.429	98	43	114	27	75	65 duplicate
17537	138 [674; Ergosterol (1TMS)]	72	[919; D-Xylopyranose (4TMS)]	45	-0.111	-0.189	13.443	0.327	99	42	115	26	48	132 duplicate
19180	138 [674; Ergosterol (1TMS)]	103	[648; Ethylamine (2TMS)]	45	-0.113	-0.205	22.362	0.399	100	41	117	24	89	86 duplicate
16069	138 [674; Ergosterol (1TMS)]	54	[NA]	38	-0.124	-0.035	12.045	0.390	101	40	101	40	38	85 duplicate
14659	138 [674; Ergosterol (1TMS)]	39	[829; 1-Phenylethanol (1TMS)]	46	-0.125	0.042	25.674	0.445	102	39	87	54	99	51 duplicate
11682	138 [674; Ergosterol (1TMS)]	13	Uracil	46	-0.129	-0.026	26.122	0.515	103	38	100	41	103	11 duplicate
15894	138 [674; Ergosterol (1TMS)]	52	[NA]	34	-0.130	-0.104	11.190	0.453	104	37	109	32	32	44 duplicate
15345	138 [674; Ergosterol (1TMS)]	46	Arabinose	46	-0.134	0.012	25.948	0.487	105	35	94	47	101	20 duplicate
16313	138 [674; Ergosterol (1TMS)]	56	[829; Orotic acid (3TMS)]	46	-0.134	-0.007	15.770	0.471	106	36	98	43	60	33 duplicate
17033	138 [674; Ergosterol (1TMS)]	65	[646; 3-Deoxyglucitol (5TMS)]	46	-0.136	0.043	18.016	0.486	107	34	85	56	73	22 duplicate
18707	138 [674; Ergosterol (1TMS)]	92	[680; Glycerol-2-phosphate (4TMS)]	46	-0.137	-0.081	14.872	0.410	108	33	105	36	54	78 duplicate
13594	138 [674; Ergosterol (1TMS)]	29	Erythritol	46	-0.144	-0.062	14.354	0.438	109	31	103	38	52	56 duplicate

18658	138 [674; Ergosterol (1TMS) 91	[766; beta-D-Methylglucopyranoside (4TMS)]	46	-0.144	-0.413	23.509	0.522	110	32	128	12	91	10 duplicate
12550	138 [674; Ergosterol (1TMS)	20											
19862	138 [674; Ergosterol (1TMS) 134	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	20	-0.147	-0.641	10.203	0.588	111	30	140	1	24	4 duplicate
13024	138 [674; Ergosterol (1TMS) 24	[725; 2-Ketooctanoic acid (2TMS)]	46	-0.150	0.022	33.832	0.457	112	29	92	49	120	43 duplicate
12060	138 [674; Ergosterol (1TMS) 16	[644; 2-Methyl-1,3-butanediol (2TMS)]	46	-0.154	-0.025	40.079	0.478	113	28	89	42	132	28 duplicate
19103	138 [674; Ergosterol (1TMS) 101	[832; Dopamine (4TMS)]	46	-0.159	-0.051	27.514	0.515	114	27	102	39	108	12 duplicate
19817	138 [674; Ergosterol (1TMS) 129	[840; Maltose methoxamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	46	-0.165	-0.369	19.202	0.393	115	28	127	14	77	91 duplicate
19838	138 [674; Ergosterol (1TMS) 131	[626; 5-Methylthioadenosine (3TMS)]	42	-0.166	0.040	18.241	0.462	116	25	88	53	74	39 duplicate
19880	138 [674; Ergosterol (1TMS) 98	[697; Ribose-5-phosphate methoxamine (5TMS)]	37	-0.168	-0.473	8.394	0.530	117	24	135	6	14	8 duplicate
12907	138 [674; Ergosterol (1TMS) 23	Homoserine	46	-0.185	-0.208	8.790	0.370	118	22	120	21	18	113 duplicate
15250	138 [674; Ergosterol (1TMS) 45	Homocysteine	46	-0.190	-0.225	17.041	0.365	119	22	121	20	64	116 duplicate
17255	138 [674; Ergosterol (1TMS) 68	[570; Hypoxanthine (2TMS)]	43	-0.192	-0.321	8.493	0.267	120	21	124	17	15	140 duplicate
16155	138 [674; Ergosterol (1TMS) 55	[612; 4-Aminobutyric acid (2TBS)]	18	-0.203	-0.196	6.259	0.331	121	20	116	25	7	131 duplicate
15982	138 [674; Ergosterol (1TMS) 53	Glycerol-2-phosphate	29	-0.212	-0.269	10.345	0.414	122	19	123	18	27	76 duplicate
	138 [674; Ergosterol (1TMS)		46	-0.214	-0.469	9.509	0.451	123	18	133	8	20	46 duplicate
16397	57	[757; 2-Deoxy-pentose-3-yose dimethoxamine (2TMS)]	38	-0.215	0.040	21.565	0.417	124	17	80	51	85	74 duplicate
13369	138 [674; Ergosterol (1TMS) 27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	38	-0.222	-0.206	13.304	0.306	125	16	119	22	47	134 duplicate
12184	138 [674; Ergosterol (1TMS) 17	[700; 2-methyl-1,2-propanediol (2TMS)]	46	-0.229	-0.104	27.416	0.447	126	15	108	33	107	49 duplicate
18837	138 [674; Ergosterol (1TMS) 97	[756; beta-D-Methylglucopyranoside (4TMS)]	36	-0.241	-0.350	28.460	0.463	127	14	126	15	110	38 duplicate
15624	138 [674; Ergosterol (1TMS) 49	[877; Pyrophosphoric acid (4TMS)]	46	-0.273	-0.395	13.285	0.420	128	13	128	13	46	71 duplicate
18287	138 [674; Ergosterol (1TMS) 84	Mannitol	44	-0.281	-0.527	39.755	0.382	129	12	138	3	131	102 duplicate
10630	138 [674; Ergosterol (1TMS) 5	Leucine	32	-0.294	-0.448	11.629	0.356	130	11	130	11	33	123 duplicate
19022	138 [674; Ergosterol (1TMS) 89	[682; Ribose-5-phosphate methoxamine (BP) (5TMS)]	34	-0.298	-0.169	10.707	0.397	131	10	113	28	30	87 duplicate
18172	138 [674; Ergosterol (1TMS) 82	Lysine	41	-0.308	-0.536	22.059	0.483	132	9	139	2	88	17 duplicate
16880	138 [674; Ergosterol (1TMS) 63	Glutamine	33	-0.318	-0.205	16.972	0.375	133	8	118	23	63	107 duplicate
15057	138 [674; Ergosterol (1TMS) 43	[548; Leucine (2TBS)]	42	-0.319	-0.472	15.363	0.461	134	7	134	7	58	41 duplicate
19253	138 [674; Ergosterol (1TMS) 105	[708; 2-Ketogluconic acid (5TMS)]	32	-0.327	-0.341	20.241	0.418	135	6	125	16	81	72 duplicate
13140	138 [674; Ergosterol (1TMS) 25	[709; 2,5-Diaminovalerolactam (2TMS)]	33	-0.352	-0.240	11.936	0.427	136	5	122	19	35	66 duplicate
18755	138 [674; Ergosterol (1TMS) 93	[607; Putrescine (4TMS)]	44	-0.353	-0.465	10.518	0.461	137	4	132	9	29	40 duplicate
15439	138 [674; Ergosterol (1TMS) 47	[NA]	46	-0.397	-0.516	17.531	0.440	138	3	137	4	68	54 duplicate
18557	138 [674; Ergosterol (1TMS) 89	[775; Dopamine (4TMS)]	29	-0.433	-0.461	15.482	0.467	139	1	131	10	59	37 duplicate
10080	138 [674; Ergosterol (1TMS) 1	[938; Sulfuric acid (2TMS)]	29	-0.433	-0.508	13.162	0.446	140	2	136	5	45	50 duplicate
18878	139 [700; Ergosta-5,7-dien-2	Ergosterol	38	0.559	0.738	26.446	0.591	1	140	2	139	97	2 duplicate
8941	139 [700; Ergosta-5,7-dien-2	[692; Ergosta-7,22-dien-3-ol (1TMS)]	37	0.556	0.725	5.336	0.509	2	139	3	138	6	4 original
9942	139 [700; Ergosta-5,7-dien-2	141 Lanosta-8,24-dien-3-beta-ol	38	0.499	0.738	10.530	0.619	3	138	1	140	20	1 original
19848	139 [700; Ergosta-5,7-dien-2	[895; Isomaltose methoxamine (8TMS)]	25	0.493	0.419	11.510	0.476	4	137	10	131	29	11 duplicate
19653	139 [700; Ergosta-5,7-dien-2	[931; myo-Inositol-2-phosphate (7TMS)]	38	0.454	0.725	20.015	0.515	5	136	4	137	76	3 duplicate
19594	139 [700; Ergosta-5,7-dien-2	[882; Pseudouridine (5TMS)]	22	0.420	0.454	12.304	0.428	6	135	9	132	32	32 duplicate
19881	139 [700; Ergosta-5,7-dien-2	[674; Ergosterol (1TMS)]	36	0.317	0.486	5.769	0.403	7	134	7	134	7	49 duplicate
19449	139 [700; Ergosta-5,7-dien-2	[583; Erythritol (4TMS)]	26	0.305	0.373	2.282	0.419	8	133	13	128	1	39 duplicate
19856	139 [700; Ergosta-5,7-dien-2	[855; Squalene]	38	0.300	0.399	19.112	0.486	9	132	12	129	68	8 duplicate
19388	139 [700; Ergosta-5,7-dien-2	109 Octadecanoic acid	38	0.263	0.200	34.600	0.410	10	131	29	112	121	44 duplicate
19631	139 [700; Ergosta-5,7-dien-2	[928; Glucopyranose-6-phosphate (6TMS)]	33	0.254	0.172	13.078	0.478	11	130	37	104	37	12 duplicate
12780	139 [700; Ergosta-5,7-dien-2	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	30	0.251	0.301	10.155	0.463	12	129	19	122	18	15 duplicate
	139 [700; Ergosta-5,7-dien-2	[734; 1-Monoolerolglycerol (2TMS); 1-Monohexadecenylglycerol (1TMS)]	38	0.249	0.549	2.905	0.425	13	128	5	136	2	35 duplicate
19748	139 [700; Ergosta-5,7-dien-2	108 Octadecenoic acid	38	0.238	0.478	15.122	0.412	14	127	8	133	49	42 duplicate
17469	139 [700; Ergosta-5,7-dien-2	71 Erythrose (3TMS)]	38	0.226	0.110	23.260	0.345	15	126	47	94	88	83 duplicate
17673	139 [700; Ergosta-5,7-dien-2	74 [912; Tetradecanoic acid (1TMS)]	38	0.223	0.220	18.864	0.297	16	125	25	116	65	114 duplicate

18803	139 [700; Ergosta-5,7-dien-3	94	Hexadecanoic acid	38	0.218	0.314	33,462	0.437	17	124	16	125	115	25 duplicate
18874	139 [700; Ergosta-5,7-dien-3	136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	14	0.209	0.413	10,681	0.281	18	123	11	130	21	122 duplicate
18644	139 [700; Ergosta-5,7-dien-3	60	Glycerol-3-phosphate	38	0.201	0.270	31,370	0.424	19	122	22	119	112	38 duplicate
19779	139 [700; Ergosta-5,7-dien-3	126	[559; Erythritol (4TMS)]	26	0.200	0.305	15,054	0.408	20	121	18	123	47	109 duplicate
18344	139 [700; Ergosta-5,7-dien-3	85	[528; Methylenic acid (4TMS)]	29	0.192	0.211	14,380	0.328	21	120	28	113	43	98 duplicate
10495	139 [700; Ergosta-5,7-dien-3	4	Phosphoric acid	30	0.186	0.217	37,825	0.281	22	119	26	115	128	121 duplicate
17183	139 [700; Ergosta-5,7-dien-3	67	Citric acid	38	0.181	0.179	32,822	0.431	23	118	34	107	114	29 duplicate
19533	139 [700; Ergosta-5,7-dien-3	114	Fructose-6-phosphate	34	0.180	0.131	13,226	0.392	24	117	44	97	39	54 duplicate
17538	139 [700; Ergosta-5,7-dien-3	72	[919; D-Xylopranose (4TMS)]	37	0.168	0.150	13,679	0.348	25	116	41	100	40	79 duplicate
18894	139 [700; Ergosta-5,7-dien-3	96	myo-Inositol	32	0.161	-0.036	3,821	0.263	26	115	82	59	3	131 duplicate
18793	139 [700; Ergosta-5,7-dien-3	127	[777; Fructose-6-phosphate methoxyamine (8TMS)]	25	0.147	0.322	14,873	0.429	27	114	14	127	44	31 duplicate
18609	139 [700; Ergosta-5,7-dien-3	90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	38	0.141	0.316	19,342	0.453	28	113	15	126	71	16 duplicate
18849	139 [700; Ergosta-5,7-dien-3	95	[770; 3,4,6-Trisubhydroxyphenylethanolamine (5TMS)]	26	0.138	0.293	6,032	0.389	29	112	21	120	9	56 duplicate
13256	139 [700; Ergosta-5,7-dien-3	26	Citramalic acid	38	0.127	0.028	26,927	0.316	30	111	64	77	101	105 duplicate
19323	139 [700; Ergosta-5,7-dien-3	107	9-(Z)-Octadecenoic acid	38	0.121	0.487	26,266	0.484	31	110	6	135	96	9 duplicate
14455	139 [700; Ergosta-5,7-dien-3	37	Phenylalanine	38	0.115	0.215	31,959	0.369	32	107	27	114	113	66 duplicate
14861	139 [700; Ergosta-5,7-dien-3	41	[639; Proline (2TMS)]	38	0.115	0.175	24,510	0.324	33	108	36	105	91	99 duplicate
19731	139 [700; Ergosta-5,7-dien-3	123	[945; Galactofuranose-6-phosphate (7TMS)]	38	0.115	-0.009	21,567	0.414	34	109	76	65	81	41 duplicate
10900	139 [700; Ergosta-5,7-dien-3	7	Threonine	38	0.110	0.154	37,576	0.341	35	108	40	101	127	89 duplicate
19869	139 [700; Ergosta-5,7-dien-3	135	[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	38	0.107	0.106	23,507	0.427	36	105	50	91	90	33 duplicate
18114	139 [700; Ergosta-5,7-dien-3	81	Tyrosine	38	0.098	0.188	40,703	0.366	37	104	31	110	135	67 duplicate
12308	139 [700; Ergosta-5,7-dien-3	18	[590; 1-Acetyl-2-thiohydantoin]	38	0.092	-0.003	19,400	0.274	38	103	72	69	73	127 duplicate
19478	139 [700; Ergosta-5,7-dien-3	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	38	0.087	0.337	6,002	0.366	39	102	60	81	8	68 duplicate
13483	139 [700; Ergosta-5,7-dien-3	28	Malic acid	38	0.084	-0.006	21,023	0.393	40	101	74	67	79	53 duplicate
19064	139 [700; Ergosta-5,7-dien-3	100	[857; Mannitol (6TMS)]	38	0.075	-0.183	20,776	0.388	41	100	94	47	78	57 duplicate
19559	139 [700; Ergosta-5,7-dien-3	115	Glucose-6-phosphate	37	0.075	-0.153	33,755	0.450	42	99	109	32	117	19 duplicate
12671	139 [700; Ergosta-5,7-dien-3	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	38	0.073	-0.004	27,278	0.285	43	98	73	68	103	120 duplicate
15895	139 [700; Ergosta-5,7-dien-3	52	[NA]	28	0.069	0.286	10,006	0.396	44	97	20	121	17	52 duplicate
18231	139 [700; Ergosta-5,7-dien-3	83	Sorbitol	33	0.068	0.036	28,813	0.337	45	96	61	80	110	93 duplicate
17868	139 [700; Ergosta-5,7-dien-3	77	[826; beta-[(5-methyl-2-thienyl)methyl]eneamino-benzeneacetic acid methyl ester]	36	0.063	0.177	36,054	0.309	46	95	35	106	124	108 duplicate
14960	139 [700; Ergosta-5,7-dien-3	42	Glutamic acid	35	0.062	0.113	34,442	0.280	47	94	46	95	120	124 duplicate
10358	139 [700; Ergosta-5,7-dien-3	3	Ethanolamine	36	0.060	0.186	12,175	0.341	48	93	32	109	31	90 duplicate
18173	139 [700; Ergosta-5,7-dien-3	82	Lysine	28	0.058	0.129	23,273	0.365	49	92	45	96	89	69 duplicate
19713	139 [700; Ergosta-5,7-dien-3	122	[644; Erythritol (4TMS)]	30	0.057	0.161	12,413	0.409	50	91	39	102	33	48 duplicate
19143	139 [700; Ergosta-5,7-dien-3	102	[904; Galactose methoxyamine (5TMS)]	38	0.055	-0.115	14,899	0.438	51	90	102	39	45	24 duplicate
13925	139 [700; Ergosta-5,7-dien-3	32	[728; N,N-Dimethyllysine methyl ester]	37	0.054	0.168	13,149	0.238	52	89	38	103	38	138 duplicate
16563	139 [700; Ergosta-5,7-dien-3	59	Ornithine; Arginine	38	0.053	0.140	45,570	0.258	53	86	43	98	138	132 duplicate
18724	139 [700; Ergosta-5,7-dien-3	61	[NA]	38	0.053	0.108	16,794	0.342	54	87	48	93	56	87 duplicate
12430	139 [700; Ergosta-5,7-dien-3	19	Alanine (BP) (3TMS)	38	0.053	-0.013	22,897	0.437	55	88	77	64	87	26 duplicate
17328	139 [700; Ergosta-5,7-dien-3	69	Arginine	35	0.052	0.098	27,867	0.370	56	85	51	90	106	65 duplicate
16070	139 [700; Ergosta-5,7-dien-3	54	[NA]	31	0.049	-0.059	12,665	0.412	57	84	88	53	35	43 duplicate
16156	139 [700; Ergosta-5,7-dien-3	55	[612; 4-Aminobutyric acid (2TBS)]	24	0.043	0.194	7,168	0.289	58	83	30	111	14	113 duplicate
19806	139 [700; Ergosta-5,7-dien-3	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	27	0.043	-0.112	18,546	0.390	59	82	100	41	64	55 duplicate
13706	139 [700; Ergosta-5,7-dien-3	30	[815; Ethyl-3(2H)-thiophenone]	38	0.041	-0.026	12,461	0.364	60	81	80	61	34	71 duplicate
11810	139 [700; Ergosta-5,7-dien-3	14	Fumaric acid	38	0.041	-0.208	14,975	0.329	62	79	126	15	46	95 duplicate
19506	139 [700; Ergosta-5,7-dien-3	113	Galactose-6-phosphate	37	0.039	-0.175	46,427	0.447	63	78	118	23	139	20 duplicate
14246	139 [700; Ergosta-5,7-dien-3	35	Pyroglutamic acid	38	0.030	-0.112	24,879	0.420	64	77	99	42	92	38 duplicate
16803	139 [700; Ergosta-5,7-dien-3	62	[812; D-Xylofuranose (4TMS)]	38	0.027	-0.112	24,879	0.420	65	75	17	124	63	135 duplicate
14033	139 [700; Ergosta-5,7-dien-3	33	Methionine	38	0.024	0.308	17,920	0.238	65	75	17	124	63	135 duplicate

15983	139 [700; Ergosta-5,7-dien-2	53	Glycerol-2-phosphate	38	0,024	0,004	10,409	0,314	66	76	71	70	19	106 duplicate
19608	139 [700; Ergosta-5,7-dien-2	117	[724; Glycerol (3TMS)]	34	0,023	0,021	17,057	0,324	67	74	67	74	60	100 duplicate
11555	139 [700; Ergosta-5,7-dien-2	12	Glyceric acid	38	0,021	-0,091	11,009	0,341	68	73	96	45	24	88 duplicate
12551	139 [700; Ergosta-5,7-dien-2	20	[619; 2-(3',4'-Bishydroxyphenyl)-2-oxethylamine (4TMS)]	18	0,020	0,063	8,714	0,476	69	72	55	86	16	13 duplicate
18708	139 [700; Ergosta-5,7-dien-2	92	[680; Glycerol-2-phosphate (4TMS)]	31	0,019	-0,249	16,100	0,381	70	71	133	8	50	60 duplicate
19694	139 [700; Ergosta-5,7-dien-2	121	[657; Erythritol (4TMS)]	33	0,015	-0,064	10,779	0,313	71	70	89	52	22	107 duplicate
16481	139 [700; Ergosta-5,7-dien-2	58	[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	38	0,010	0,017	25,224	0,307	72	69	68	73	93	110 duplicate
17256	139 [700; Ergosta-5,7-dien-2	68	[570; Hypoxanthine (2TMS)]	15	0,010	0,264	4,598	0,247	73	68	23	118	4	134 duplicate
14351	139 [700; Ergosta-5,7-dien-2	36	[596; N-Acetylglutamic acid (2TMS)]	38	0,007	-0,025	36,260	0,301	74	67	79	62	125	112 duplicate
18054	139 [700; Ergosta-5,7-dien-2	80	[772; D-Glucose (5TMS)]	36	0,000	-0,122	35,200	0,278	75	66	103	38	122	125 duplicate
19674	139 [700; Ergosta-5,7-dien-2	120	[945; Uridine (3TMS)]	32	-0,004	-0,109	22,213	0,318	76	65	98	43	83	103 duplicate
11426	139 [700; Ergosta-5,7-dien-2	11	Succinic acid	38	-0,013	-0,156	19,315	0,404	77	64	113	28	70	47 duplicate
19419	139 [700; Ergosta-5,7-dien-2	110	[715; Erythritol (4TMS)]	31	-0,015	-0,051	18,819	0,404	78	63	85	56	57	48 duplicate
19764	139 [700; Ergosta-5,7-dien-2	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	38	-0,016	-0,222	38,187	0,349	79	62	130	11	129	77 duplicate
13370	139 [700; Ergosta-5,7-dien-2	27	[815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	30	-0,016	0,025	11,201	0,223	80	61	65	76	28	138 duplicate
19818	139 [700; Ergosta-5,7-dien-2	129	[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]	34	-0,020	0,039	19,367	0,506	81	60	58	83	72	5 duplicate
11165	139 [700; Ergosta-5,7-dien-2	9	Proline	38	-0,021	0,106	33,507	0,273	82	59	49	92	116	128 duplicate
16958	139 [700; Ergosta-5,7-dien-2	64	[788; Tyramine (3TMS)]	37	-0,024	-0,236	15,058	0,410	83	58	132	9	48	45 duplicate
15806	139 [700; Ergosta-5,7-dien-2	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	26	-0,028	0,081	6,519	0,316	84	57	53	88	10	104 duplicate
18756	139 [700; Ergosta-5,7-dien-2	93	[907; Putrescine (4TMS)]	36	-0,029	0,032	8,530	0,345	85	58	63	78	15	82 duplicate
10220	139 [700; Ergosta-5,7-dien-2	2	Serine	36	-0,032	0,184	25,472	0,365	86	55	33	108	94	70 duplicate
15251	139 [700; Ergosta-5,7-dien-2	45	Homocysteine	35	-0,032	-0,007	5,149	0,235	87	54	75	66	5	137 duplicate
17739	139 [700; Ergosta-5,7-dien-2	85	Lysine	38	-0,033	0,071	44,631	0,285	88	53	54	87	137	119 duplicate
18288	139 [700; Ergosta-5,7-dien-2	84	Mannitol	36	-0,035	-0,058	38,260	0,348	89	52	87	54	130	78 duplicate
15716	139 [700; Ergosta-5,7-dien-2	50	[746; Ribonic acid-1,4-lactone (3TMS)]	35	-0,035	-0,067	6,607	0,357	90	50	91	50	11	73 duplicate
17399	139 [700; Ergosta-5,7-dien-2	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	35	-0,035	-0,215	27,484	0,280	91	51	127	14	105	123 duplicate
15058	139 [700; Ergosta-5,7-dien-2	43	[548; Leucine (2TBS)]	35	-0,039	-0,036	16,525	0,343	92	49	83	58	52	86 duplicate
19181	139 [700; Ergosta-5,7-dien-2	103	[648; Ethylamine (2TMS)]	37	-0,039	-0,144	22,524	0,321	93	48	106	35	85	101 duplicate
16398	139 [700; Ergosta-5,7-dien-2	57	[757; 2-Desoxy-pentos-3-ylose dimethoxyamine (2TMS)]	30	-0,039	-0,064	22,419	0,441	94	47	90	51	84	23 duplicate
19828	139 [700; Ergosta-5,7-dien-2	130	Trehalose	37	-0,042	0,053	37,142	0,421	95	46	56	85	126	37 duplicate
19254	139 [700; Ergosta-5,7-dien-2	105	[705; 2-Ketogluconic acid (5TMS)]	26	-0,046	0,038	20,318	0,327	96	45	59	82	77	97 duplicate
14140	139 [700; Ergosta-5,7-dien-2	34	Aspartic acid	38	-0,047	0,148	38,508	0,249	97	44	42	99	131	133 duplicate
19839	139 [700; Ergosta-5,7-dien-2	131	[626; 5-Methylthioadenosine (3TMS)]	30	-0,048	-0,027	6,930	0,297	98	43	81	60	12	115 duplicate
15155	139 [700; Ergosta-5,7-dien-2	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	27	-0,048	-0,068	19,858	0,385	99	42	92	49	75	59 duplicate
16314	139 [700; Ergosta-5,7-dien-2	56	[828; Orolic acid (3TMS)]	38	-0,055	-0,159	16,899	0,467	100	41	115	26	59	14 duplicate
11298	139 [700; Ergosta-5,7-dien-2	10	Glycine	38	-0,061	0,046	27,792	0,426	101	40	57	84	107	34 duplicate
19289	139 [700; Ergosta-5,7-dien-2	106	[733; Threitol (4TMS)]	37	-0,066	-0,218	21,326	0,437	102	39	129	12	80	27 duplicate
14761	139 [700; Ergosta-5,7-dien-2	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	38	-0,067	-0,155	41,442	0,357	103	37	111	30	136	74 duplicate
11936	139 [700; Ergosta-5,7-dien-2	15	Alanine	38	-0,067	-0,264	26,551	0,371	104	38	135	6	98	64 duplicate
10631	139 [700; Ergosta-5,7-dien-2	5	Leucine	27	-0,071	0,034	11,678	0,128	105	36	62	79	30	140 duplicate
18453	139 [700; Ergosta-5,7-dien-2	87	[945; beta-D-Glucopyranose (5TMS)]	37	-0,072	-0,143	40,207	0,386	106	34	105	36	133	58 duplicate
17034	139 [700; Ergosta-5,7-dien-2	65	[646; 3-Deoxyglucitol (5TMS)]	37	-0,072	-0,153	19,093	0,502	107	35	110	31	67	6 duplicate
15440	139 [700; Ergosta-5,7-dien-2	47	[NA]	38	-0,073	-0,108	16,878	0,359	108	33	97	44	58	72 duplicate
15625	139 [700; Ergosta-5,7-dien-2	49	[877; Pyrophosphoric acid (4TMS)]	38	-0,075	0,008	11,196	0,271	109	32	70	71	25	130 duplicate
16881	139 [700; Ergosta-5,7-dien-2	63	Glutamine	36	-0,079	0,094	16,547	0,398	110	31	52	89	53	51 duplicate
14558	139 [700; Ergosta-5,7-dien-2	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	38	-0,084	-0,155	19,509	0,380	111	29	112	29	74	62 duplicate
19863	139 [700; Ergosta-5,7-dien-2	134	isomaltose	38	-0,084	-0,159	34,246	0,446	112	30	114	27	118	21 duplicate

19218	139 [700; Ergosta-5,7-dien-2	104	[795; Erythritol (4TMS)]	37	-0,084	-0,275	17,463	0,345	113	28	137	4	61	84 duplicate
18506	139 [700; Ergosta-5,7-dien-2	88	Gluconic acid	38	-0,087	-0,114	22,852	0,431	114	26	101	40	86	30 duplicate
11683	139 [700; Ergosta-5,7-dien-2	13	Uracil	38	-0,087	-0,148	27,081	0,450	115	27	107	34	102	17 duplicate
17804	139 [700; Ergosta-5,7-dien-2	76	Fructose	38	-0,101	-0,216	34,334	0,398	116	25	128	13	119	50 duplicate
18981	139 [700; Ergosta-5,7-dien-2	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	26	-0,114	-0,089	7,008	0,200	117	24	95	48	13	139 duplicate
18399	139 [700; Ergosta-5,7-dien-2	86	[793; D-Galactono-1,4-lactone (4TMS)]	37	-0,114	-0,200	30,462	0,495	118	23	122	19	111	7 duplicate
17993	139 [700; Ergosta-5,7-dien-2	79	Glucose	38	-0,118	-0,261	40,242	0,335	119	21	134	7	134	94 duplicate
19104	139 [700; Ergosta-5,7-dien-2	101	[832; Dopamine (4TMS)]	38	-0,118	-0,272	19,190	0,347	120	22	136	5	89	80 duplicate
17606	139 [700; Ergosta-5,7-dien-2	73	[708; Glucose methoxyamine (5TMS)]	35	-0,119	-0,190	16,761	0,305	121	20	120	21	55	111 duplicate
10081	139 [700; Ergosta-5,7-dien-2	31	[938; Sulfuric acid (2TMS)]	25	-0,120	-0,400	13,035	0,288	122	19	84	57	38	118 duplicate
18938	139 [700; Ergosta-5,7-dien-2	97	[756; beta-D-Methylglucopyranoside (4TMS)]	30	-0,122	-0,173	27,412	0,293	123	18	116	25	104	116 duplicate
15346	139 [700; Ergosta-5,7-dien-2	46	Arabinose	38	-0,124	-0,191	26,746	0,481	124	16	121	20	100	10 duplicate
18659	139 [700; Ergosta-5,7-dien-2	91	[766; beta-D-Methylglucopyranoside (4TMS)]	38	-0,124	-0,205	21,985	0,319	125	17	124	17	82	102 duplicate
17931	139 [700; Ergosta-5,7-dien-2	78	Mannose	38	-0,127	-0,174	16,697	0,354	126	15	117	24	64	75 duplicate
17109	139 [700; Ergosta-5,7-dien-2	66	Glyceric acid-3-phosphate	38	-0,129	-0,177	14,228	0,325	127	14	119	22	42	98 duplicate
19023	139 [700; Ergosta-5,7-dien-2	99	[682; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	29	-0,133	-0,056	11,460	0,338	128	13	86	55	28	92 duplicate
13816	139 [700; Ergosta-5,7-dien-2	31	[622; Parabenic acid (2TMS)]	38	-0,144	-0,152	11,324	0,293	129	12	108	33	27	117 duplicate
11033	139 [700; Ergosta-5,7-dien-2	3	Isoleucine	31	-0,144	0,022	25,504	0,350	130	11	66	75	95	76 duplicate
13025	139 [700; Ergosta-5,7-dien-2	84	[725; 2-Ketotolanoic acid (2TMS)]	38	-0,149	-0,204	39,876	0,441	131	10	123	18	132	22 duplicate
15533	139 [700; Ergosta-5,7-dien-2	48	Asparagine	38	-0,158	0,014	19,071	0,416	132	9	69	72	66	40 duplicate
12061	139 [700; Ergosta-5,7-dien-2	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	38	-0,164	-0,206	28,370	0,450	133	8	125	16	109	18 duplicate
18558	139 [700; Ergosta-5,7-dien-2	89	[775; Dopamine (4TMS)]	24	-0,167	-0,017	13,683	0,344	134	7	78	63	41	85 duplicate
13595	139 [700; Ergosta-5,7-dien-2	29	Erythritol	38	-0,169	-0,224	16,132	0,345	135	6	131	10	51	81 duplicate
12808	139 [700; Ergosta-5,7-dien-2	23	Homoserine	38	-0,181	-0,082	17,602	0,274	136	5	93	48	62	126 duplicate
12185	139 [700; Ergosta-5,7-dien-2	17	[700; 2-methyl-1,2-propanediol (2TMS)]	38	-0,209	-0,335	28,347	0,390	137	4	138	3	108	61 duplicate
14660	139 [700; Ergosta-5,7-dien-2	39	[829; 1-Phenylethanol (1TMS)]	37	-0,218	-0,142	26,612	0,431	138	3	104	37	99	28 duplicate
10766	139 [700; Ergosta-5,7-dien-2	6	Glycerol	38	-0,272	-0,379	46,474	0,338	139	2	140	1	140	91 duplicate
13141	139 [700; Ergosta-5,7-dien-2	25	[709; 2,5-Diaminovalerolactam (2TMS)]	27	-0,305	-0,337	10,910	0,374	140	1	139	2	23	63 duplicate
9943	140 [692; Ergosta-7,22-dien-	141	Lanosta-8,24-dien-3-beta-ol	49	0,828	0,969	5,933	0,706	1	141	1	141	7	1 original
19879	140 [692; Ergosta-7,22-dien-	137	Ergosterol	49	0,793	0,947	24,183	0,621	2	140	2	140	86	2 duplicate
19882	140 [692; Ergosta-7,22-dien-	138	[674; Ergosterol (1TMS)]	43	0,661	0,810	2,687	0,601	3	139	3	139	1	3 duplicate
19389	140 [692; Ergosta-7,22-dien-	109	Octadecanoic acid	49	0,614	0,617	32,289	0,480	4	138	11	131	117	20 duplicate
19585	140 [692; Ergosta-7,22-dien-	132	[892; Pseudouridine (5TMS)]	29	0,606	0,633	9,382	0,456	5	137	9	133	27	36 duplicate
19849	140 [692; Ergosta-7,22-dien-	94	Hexadecanoic acid	33	0,595	0,736	9,381	0,407	6	136	4	138	26	84 duplicate
18804	140 [692; Ergosta-7,22-dien-	139	[700; Ergosta-5,7-dien-3-ol]	49	0,568	0,686	31,699	0,540	7	135	7	135	114	6 duplicate
19884	140 [692; Ergosta-7,22-dien-	139	[700; Ergosta-5,7-dien-3-ol]	37	0,556	0,725	5,336	0,509	8	134	5	137	6	8 duplicate
17674	140 [692; Ergosta-7,22-dien-	74	[912; Tetradecanoic acid (1TMS)]	49	0,515	0,615	14,989	0,461	9	133	12	130	59	32 duplicate
19780	140 [692; Ergosta-7,22-dien-	126	[559; Erythritol (4TMS)]	32	0,504	0,719	11,338	0,428	10	132	6	136	36	63 duplicate
18345	140 [692; Ergosta-7,22-dien-	85	[528; Methylcitric acid (4TMS)]	40	0,477	0,620	12,233	0,492	11	131	10	132	40	14 duplicate
18857	140 [692; Ergosta-7,22-dien-	133	[855; Squalene]	49	0,461	0,516	16,510	0,573	12	130	16	126	68	4 duplicate
19654	140 [692; Ergosta-7,22-dien-	119	[931; myo-Inositol-2-phosphate (7TMS)]	49	0,415	0,650	17,272	0,496	13	129	8	134	75	10 duplicate
19714	140 [692; Ergosta-7,22-dien-	122	[844; Erythritol (4TMS)]	37	0,405	0,561	9,347	0,418	14	128	13	129	25	75 duplicate
15156	140 [692; Ergosta-7,22-dien-	44	[910; 2-Ketogluconic acid methoxyamine (4TMS)]	35	0,402	0,541	16,738	0,425	15	127	14	128	73	65 duplicate
18450	140 [692; Ergosta-7,22-dien-	111	[583; Erythritol (4TMS)]	32	0,383	0,539	4,932	0,472	16	126	15	127	3	26 duplicate
12791	140 [692; Ergosta-7,22-dien-	22	[690; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	38	0,351	0,473	6,776	0,418	17	125	17	125	10	74 duplicate
19534	140 [692; Ergosta-7,22-dien-	114	Fructose-6-phosphate	42	0,336	0,354	9,833	0,408	18	124	29	113	30	85 duplicate
19065	140 [692; Ergosta-7,22-dien-	100	[857; Mannitol (6TMS)]	49	0,327	0,344	18,264	0,395	19	123	31	111	78	88 duplicate
19749	140 [692; Ergosta-7,22-dien-	124	[734; 1-Monooctylethylglycerol (2TMS); 1-Monohexadecanoylglycerol (1TMS)]	47	0,323	0,449	6,194	0,439	20	122	20	122	8	53 duplicate
19870	140 [692; Ergosta-7,22-dien-	135	[902; Melibiose (8TMS); alpha-D-Gal(1,6)-D-Glc (8TMS)]	49	0,298	0,458	21,725	0,484	21	121	19	123	89	17 duplicate

18609	140 [692; Ergosta-7,22-dien-117	1724; Glycerol (3TMS)]	42	0.296	0.441	13.481	0.381	22	120	21	121	49	105 duplicate
17470	140 [692; Ergosta-7,22-dien-71	[731; Erythrose (3TMS)]	49	0.293	0.214	21.819	0.407	23	119	50	92	90	83 duplicate
18695	140 [692; Ergosta-7,22-dien-121	[657; Erythritol (4TMS)]	41	0.288	0.393	7.605	0.391	24	118	24	118	16	94 duplicate
18895	140 [692; Ergosta-7,22-dien-96	myo-Inositol	42	0.287	0.395	5.140	0.338	25	117	23	119	4	133 duplicate
19560	140 [692; Ergosta-7,22-dien-115	Glucose-6-phosphate	47	0.286	0.180	32.369	0.448	26	116	57	85	118	43 duplicate
19420	140 [692; Ergosta-7,22-dien-110	[715; Erythritol (4TMS)]	39	0.282	0.323	13.704	0.523	27	115	35	107	51	7 duplicate
12309	140 [692; Ergosta-7,22-dien-18	[590; 1-Acetyl-2-thiohydantoin]	49	0.274	0.338	16.828	0.408	28	114	32	110	74	82 duplicate
13484	140 [692; Ergosta-7,22-dien-28	Malic acid	49	0.272	0.365	18.578	0.451	29	113	27	115	80	41 duplicate
19144	140 [692; Ergosta-7,22-dien-102	[904; Galactose methoxamine (5TMS)]	49	0.269	0.282	11.785	0.460	30	112	40	102	38	33 duplicate
19479	140 [692; Ergosta-7,22-dien-112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	48	0.246	0.289	3.251	0.447	31	111	39	103	2	44 duplicate
13257	140 [692; Ergosta-7,22-dien-26	Citramalic acid	49	0.243	0.372	25.557	0.394	32	110	28	116	101	90 duplicate
12672	140 [692; Ergosta-7,22-dien-21	[678; N,N-DI-(2-Hydroxyethyl)-methanamine (2TMS)]	49	0.223	0.350	25.634	0.418	33	109	30	112	102	73 duplicate
14762	140 [692; Ergosta-7,22-dien-40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	49	0.223	0.302	22.800	0.404	34	107	34	108	136	76 duplicate
14862	140 [692; Ergosta-7,22-dien-41	[639; Proline (2TMS)]	49	0.219	0.336	8.878	0.441	35	108	38	104	91	86 duplicate
11811	140 [692; Ergosta-7,22-dien-14	Fumaric acid	49	0.218	0.306	30.867	0.414	36	106	37	105	113	48 duplicate
16645	140 [692; Ergosta-7,22-dien-60	Glycerol-3-phosphate	49	0.211	0.469	24.661	0.420	37	105	37	105	113	79 duplicate
19324	140 [692; Ergosta-7,22-dien-107	9-(Z)-Octadecanoic acid	48	0.204	0.234	18.454	0.490	38	104	18	124	98	71 duplicate
19290	140 [692; Ergosta-7,22-dien-106	[733; Threitol (4TMS)]	49	0.184	0.203	20.836	0.455	39	103	47	95	79	16 duplicate
12431	140 [692; Ergosta-7,22-dien-19	Alanine (BP) (3TMS)	29	0.187	0.355	10.987	0.440	40	102	52	90	88	39 duplicate
19794	140 [692; Ergosta-7,22-dien-127	[777; Fructose-6-phosphate methoxamine (6TMS)]	48	0.186	0.268	7.335	0.423	41	101	28	114	34	50 duplicate
11556	140 [692; Ergosta-7,22-dien-12	Glycic acid	47	0.186	0.078	12.025	0.348	42	100	44	98	14	66 duplicate
19507	140 [692; Ergosta-7,22-dien-113	Galactose-6-phosphate	44	0.171	0.055	29.389	0.400	43	99	80	62	39	124 duplicate
18232	140 [692; Ergosta-7,22-dien-83	Sorbitol	49	0.170	0.119	33.194	0.469	44	98	83	59	111	87 duplicate
17805	140 [692; Ergosta-7,22-dien-76	Fructose	49	0.168	0.392	16.600	0.369	45	97	71	71	120	29 duplicate
18610	140 [692; Ergosta-7,22-dien-90	[910; 9-(Z)-Hexadecenoic acid (1TMS)]	40	0.162	0.100	20.131	0.393	46	96	25	117	69	114 duplicate
18675	140 [692; Ergosta-7,22-dien-120	[945; Uridine (3TMS)]	49	0.155	0.112	19.908	0.440	47	95	74	68	87	93 duplicate
19732	140 [692; Ergosta-7,22-dien-123	[945; Galactofuranose-6-phosphate (7TMS)]	49	0.151	0.118	23.219	0.425	48	94	73	69	85	52 duplicate
16804	140 [692; Ergosta-7,22-dien-62	[812; D-Xylofuranose (4TMS)]	49	0.145	0.136	32.747	0.422	49	93	72	70	92	64 duplicate
17184	140 [692; Ergosta-7,22-dien-67	Citric acid	49	0.144	0.084	26.653	0.300	50	92	66	78	119	69 duplicate
17400	140 [692; Ergosta-7,22-dien-70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	46	0.143	0.024	47.771	0.440	51	91	68	76	119	140 duplicate
14247	140 [692; Ergosta-7,22-dien-35	Pyrogulamic acid	49	0.141	0.282	12.487	0.446	52	90	78	64	108	51 duplicate
19357	140 [692; Ergosta-7,22-dien-108	Octadecanoic acid	49	0.126	0.121	15.208	0.450	53	89	86	58	139	45 duplicate
16071	140 [692; Ergosta-7,22-dien-54	[NA]	40	0.125	0.220	9.886	0.355	54	88	42	100	43	42 duplicate
15717	140 [692; Ergosta-7,22-dien-50	[746; Ribonic acid-1,4-lactone (3TMS)]	46	0.125	0.286	5.167	0.429	55	87	70	72	61	122 duplicate
19875	140 [692; Ergosta-7,22-dien-136	[748; D-Sedoheptulose-7-phosphate (7TMS)]	14	0.121	0.201	7.454	0.344	56	86	49	83	31	59 duplicate
11427	140 [692; Ergosta-7,22-dien-11	Succinic acid	49	0.121	0.183	16.674	0.390	57	85	41	101	5	130 duplicate
19255	140 [692; Ergosta-7,22-dien-105	[705; 2-Ketogluconic acid (5TMS)]	33	0.114	0.401	16.661	0.388	58	84	53	89	15	95 duplicate
17932	140 [692; Ergosta-7,22-dien-78	Mannose	49	0.111	0.135	13.874	0.455	59	83	55	87	72	98 duplicate
16399	140 [692; Ergosta-7,22-dien-57	[757; 2-Desoxy-pentose-3-ylose dimethoxamine (2TMS)]	49	0.108	0.321	19.507	0.434	60	82	22	120	71	38 duplicate
18632	140 [692; Ergosta-7,22-dien-118	[928; Glucopyranose-6-phosphate (6TMS)]	40	0.108	0.321	19.507	0.434	61	81	67	75	54	54 duplicate
19807	140 [692; Ergosta-7,22-dien-128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	43	0.103	0.011	11.479	0.463	62	80	36	106	84	31 duplicate
18709	140 [692; Ergosta-7,22-dien-92	[680; Glycerol-2-phosphate (4TMS)]	31	0.097	0.158	15.025	0.379	63	79	90	52	37	108 duplicate
19765	140 [692; Ergosta-7,22-dien-125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	39	0.096	0.011	13.801	0.331	64	78	62	80	60	136 duplicate
19819	140 [692; Ergosta-7,22-dien-129	Glc	49	0.075	-0.027	38.447	0.379	65	77	89	53	53	110 duplicate
14559	140 [692; Ergosta-7,22-dien-38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	44	0.072	0.253	16.272	0.483	66	76	97	45	128	18 duplicate
11684	140 [692; Ergosta-7,22-dien-13	Uracil	49	0.071	0.244	16.601	0.417	67	75	45	97	66	77 duplicate
19864	140 [692; Ergosta-7,22-dien-134	Isomaltose	49	0.063	0.230	24.466	0.494	68	74	46	96	70	12 duplicate
14352	140 [692; Ergosta-7,22-dien-36	[596; N-Acetylglutamic acid (2TMS)]	49	0.046	0.171	32.093	0.477	69	73	48	94	97	21 duplicate
			49	0.043	0.023	37.293	0.393	70	72	59	83	116	92 duplicate
								71	71	87	55	123	

17035	140 [692; Ergosta-7,22-dien-140 [692; Ergosta-7,22-dien-	65	[646; 3-Deoxyglucitol (5TMS)]	48	0,041	0,205	16,073	0,473	72	70	51	91	64	25-juplicate
12552	20 [619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]	25	0,040	-0,076	9,170	0,545	73	69	105	37	24	5-juplicate		
18507	88 Gluconic acid	49	0,037	0,170	19,948	0,483	74	68	60	82	86	19-juplicate		
14661	39 [829; 1-Phenylethanol (1TMS)]	48	0,037	0,279	23,527	0,446	75	68	43	99	93	48-juplicate		
18400	86 [793; D-Galactono-1,4-lactone (4TMS)]	48	0,037	0,092	28,352	0,487	76	67	76	68	109	9-juplicate		
17607	73 [708; Glucose methoxamine (5TMS)]	46	0,034	0,138	13,971	0,348	77	65	65	77	55	125-juplicate		
10359	3 Ethanolamine	47	0,031	0,085	10,573	0,374	78	64	77	65	33	112-juplicate		
13598	29 Erythritol	49	0,029	0,181	13,141	0,441	79	62	56	86	47	47-juplicate		
16315	56 [829; Orotic acid (3TMS)]	49	0,029	0,146	13,765	0,467	80	63	64	78	52	30-juplicate		
19182	103 [648; Ethylamine (2TMS)]	48	0,028	0,100	19,260	0,387	81	61	75	67	82	100-juplicate		
18850	95 [770; 3,4,6-Trisubstitutedphenylethanolamine (5TMS)]	36	0,025	0,133	7,074	0,415	82	60	68	74	12	78-juplicate		
15347	46 Arabinose	49	0,015	0,126	24,056	0,491	83	59	69	73	95	15-juplicate		
14456	37 Phenylethanol	49	0,007	0,013	31,925	0,408	84	58	88	54	115	80-juplicate		
18939	97 [756; beta-D-Methylglucopyranoside (4TMS)]	37	0,000	0,008	24,924	0,328	85	57	91	51	99	137-juplicate		
18289	84 Mannitol	47	-0,001	0,036	37,508	0,344	86	56	85	57	125	131-juplicate		
12062	16 [644; 2-Methyl-1,3-butanediol (2TMS)]	49	-0,002	0,184	26,392	0,494	87	55	54	88	105	13-juplicate		
18454	87 [945; beta-D-Glucopyranose (5TMS)]	48	-0,005	-0,018	41,160	0,358	88	53	94	48	134	121-juplicate		
17539	72 [919; D-Xylopyranose (4TMS)]	48	-0,005	-0,078	12,481	0,346	89	54	108	38	42	128-juplicate		
13026	24 [725; 2-Ketooctanoic acid (2TMS)]	49	-0,019	0,160	39,326	0,474	90	52	61	81	131	23-juplicate		
19830	130 Trehalose	48	-0,021	-0,043	37,966	0,370	91	51	98	44	127	113-juplicate		
18115	81 Tyrosine	49	-0,024	-0,018	42,768	0,422	92	50	95	47	137	68-juplicate		
17869	77 [826; beta-[[5-methyl-2-thienyl(methyl)amino]-benzenecarboxylic acid methyl ester]	47	-0,025	-0,054	38,075	0,378	93	49	99	43	128	111-juplicate		
10901	7 Threonine	49	-0,026	-0,074	38,467	0,419	94	48	103	39	130	72-juplicate		
16482	58 [636; 4R-Acetamido-2,3-(2'-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	49	-0,041	-0,134	25,006	0,398	95	47	112	30	100	88-juplicate		
10498	4 Phosphoric acid	41	-0,041	0,000	40,588	0,381	96	46	92	50	133	106-juplicate		
10767	6 Glycerol	49	-0,043	-0,092	47,943	0,348	97	45	109	33	141	126-juplicate		
18055	80 [772; D-Glucose (5TMS)]	47	-0,047	-0,090	36,265	0,317	98	44	108	34	122	139-juplicate		
12188	17 [700; 2-methyl-1,2-propanediol (2TMS)]	49	-0,053	0,068	26,083	0,380	99	43	81	61	103	107-juplicate		
18660	91 [766; beta-D-Methylglucopyranoside (4TMS)]	49	-0,054	-0,068	19,377	0,433	100	42	101	41	83	55-juplicate		
14961	42 Glutamic acid	45	-0,081	-0,167	37,361	0,432	101	41	117	25	124	58-juplicate		
17740	75 Lysine	49	-0,065	-0,075	46,765	0,347	102	40	104	38	138	128-juplicate		
15998	52 [NA]	35	-0,066	0,053	11,082	0,427	103	39	84	58	35	62-juplicate		
16959	84 [789; Tyramine (3TMS)]	48	-0,073	-0,098	12,607	0,394	104	38	110	32	44	91-juplicate		
16564	59 Ornithine; Arginine	49	-0,080	-0,160	47,913	0,364	105	37	116	26	140	119-juplicate		
17994	79 Glucose	49	-0,082	-0,126	41,445	0,344	106	36	111	31	135	132-juplicate		
16157	55 [612; 4-Aminobutyric acid (2TBS)]	55	-0,086	0,079	9,717	0,384	107	35	79	63	28	102-juplicate		
18757	93 [607; Putrescine (4TMS)]	34	-0,084	-0,008	7,279	0,430	108	34	93	49	13	57-juplicate		
19105	101 [832; Dopamine (4TMS)]	47	-0,086	-0,068	16,165	0,388	109	33	100	42	65	97-juplicate		
16725	61 [NA]	49	-0,095	-0,018	14,634	0,333	110	32	96	46	57	135-juplicate		
15984	53 Glycerol-2-phosphate	49	-0,100	-0,192	8,087	0,429	111	30	119	23	20	60-juplicate		
11937	15 Alanine	49	-0,105	-0,250	26,313	0,421	112	31	126	16	104	70-juplicate		
15907	51 [499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	35	-0,116	-0,144	8,210	0,368	113	29	114	28	21	115-juplicate		
17329	69 Arginine	48	-0,123	-0,263	29,612	0,472	114	28	127	15	112	27-juplicate		
10082	1 [938; Sulfuric acid (2TMS)]	26	-0,132	0,058	9,968	0,327	115	27	82	60	32	138-juplicate		
19024	99 [682; Ribose-5-phosphate methoxamine (BP) (5TMS)]	32	-0,133	0,178	8,046	0,451	116	26	58	84	19	40-juplicate		
18174	82 Lysine	35	-0,170	-0,270	23,808	0,474	117	25	128	14	94	24-juplicate		
11297	10 Glycine	49	-0,170	-0,246	28,406	0,471	118	24	125	17	110	28-juplicate		
13926	32 [729; N,N-Dimethyllysine methyl ester]	48	-0,177	-0,243	14,533	0,456	119	23	123	19	56	37-juplicate		



15441	140 [692; Ergosta-7,22-dien-47 [NA]	49	-0.182	-0.273	15.661	0.361	120	22	129	13	62	120 duplicate
19840	140 [692; Ergosta-7,22-dien-131 [626; 5-Methylthioadenosine (3TMS)]	40	-0.182	-0.290	7.066	0.459	121	21	131	11	11	34 duplicate
13707	140 [692; Ergosta-7,22-dien-30 [815; Ethyl-3(2H)-thiophenone]	40	-0.192	-0.221	37.836	0.350	122	20	121	21	126	123 duplicate
10632	140 [692; Ergosta-7,22-dien-5 Leucine	38	-0.198	-0.331	12.627	0.379	123	19	134	8	45	108 duplicate
15534	140 [692; Ergosta-7,22-dien-48 Asparagine	49	-0.201	-0.207	18.860	0.475	124	18	120	22	81	22 duplicate
17257	140 [692; Ergosta-7,22-dien-68 [570; Hypoxanthine (2TMS)]	19	-0.205	-0.178	6.419	0.388	125	17	118	24	9	99 duplicate
14034	140 [692; Ergosta-7,22-dien-33 Methionine	49	-0.211	-0.226	18.050	0.366	126	16	122	20	76	116 duplicate
11166	140 [692; Ergosta-7,22-dien-9 Proline	49	-0.219	-0.140	35.600	0.384	127	15	113	29	121	101 duplicate
10221	140 [692; Ergosta-7,22-dien-2 Serine	47	-0.230	-0.070	26.547	0.408	128	14	102	40	107	81 duplicate
15252	140 [692; Ergosta-7,22-dien-45 Homocysteine	46	-0.231	-0.295	7.676	0.298	129	13	132	10	17	141 duplicate
16882	140 [692; Ergosta-7,22-dien-63 Glutamine	43	-0.236	-0.078	16.495	0.389	130	11	107	35	67	98 duplicate
13817	140 [692; Ergosta-7,22-dien-31 [622; Parabenic acid (2TMS)]	49	-0.259	-0.360	9.828	0.430	131	11	135	7	29	58 duplicate
14141	140 [692; Ergosta-7,22-dien-34 Aspartic acid	49	-0.260	-0.321	40.552	0.337	132	10	133	9	132	134 duplicate
17110	140 [692; Ergosta-7,22-dien-66 Glycine acid-3-phosphate	49	-0.264	-0.273	12.313	0.440	133	9	130	12	41	49 duplicate
15059	140 [692; Ergosta-7,22-dien-43 [548; Leucine (2TBS)]	46	-0.266	-0.419	15.878	0.383	134	8	139	3	63	104 duplicate
15826	140 [692; Ergosta-7,22-dien-49 [877; Pyrophosphoric acid (4TMS)]	49	-0.284	-0.386	13.080	0.364	135	7	137	5	46	117 duplicate
11034	140 [692; Ergosta-7,22-dien-8 Isoleucine	42	-0.298	-0.150	26.403	0.428	136	6	115	27	106	61 duplicate
18559	140 [692; Ergosta-7,22-dien-89 [775; Dopamine (4TMS)]	30	-0.329	-0.245	14.774	0.459	137	5	124	18	58	35 duplicate
13371	140 [692; Ergosta-7,22-dien-27 [815; (E)-4-Methyl-5-hydroxy-3-penten-2-one (1TMS)]	40	-0.356	-0.397	13.626	0.364	138	4	138	4	50	118 duplicate
18982	140 [692; Ergosta-7,22-dien-98 [697; Ribose-5-phosphate methoxyamine (5TMS)]	34	-0.401	-0.386	8.570	0.383	139	3	136	6	22	103 duplicate
12909	140 [692; Ergosta-7,22-dien-23 Homoserine	49	-0.405	-0.473	18.251	0.422	140	2	140	2	77	67 duplicate
13142	140 [692; Ergosta-7,22-dien-25 [709; 2,5-Diaminovalerolactam (2TMS)]	33	-0.455	-0.624	13.182	0.494	141	1	141	1	48	11 duplicate
19880	141 Lanosta-8,24-dien-3-bet 137 Ergosterol	61	0.881	0.983	20.588	0.669	1	141	1	141	90	2 duplicate
19886	141 Lanosta-8,24-dien-3-bet 140 [692; Ergosta-7,22-dien-3-ol (1TMS)]	49	0.828	0.969	5.933	0.706	2	140	2	140	2	1 duplicate
19883	141 Lanosta-8,24-dien-3-bet 138 [674; Ergosterol (1TMS)]	45	0.731	0.867	6.570	0.644	3	139	3	139	4	3 duplicate
19390	141 Lanosta-8,24-dien-3-bet 109 Octadecanoic acid	61	0.875	0.674	29.209	0.570	4	138	10	132	113	6 duplicate
18805	141 Lanosta-8,24-dien-3-bet 94 Hexadecanoic acid	61	0.668	0.759	29.190	0.603	5	137	7	135	112	5 duplicate
19586	141 Lanosta-8,24-dien-3-bet 116 [882; Pseudouridine (5TMS)]	30	0.837	0.792	6.085	0.528	6	136	4	138	3	9 duplicate
19655	141 Lanosta-8,24-dien-3-bet 119 [931; myo-Inositol-2-phosphate (7TMS)]	61	0.584	0.792	13.565	0.514	7	135	5	137	54	17 duplicate
19781	141 Lanosta-8,24-dien-3-bet 126 [559; Erythritol (4TMS)]	42	0.538	0.777	8.384	0.537	8	134	6	136	11	8 duplicate
19885	141 Lanosta-8,24-dien-3-bet 139 [700; Ergosta-5,7-dien-3-ol]	38	0.499	0.738	10.530	0.619	9	133	8	134	31	4 duplicate
19750	141 Lanosta-8,24-dien-3-bet 124 Monohexadecanoylglycerol (2TMS); 1-	56	0.486	0.619	11.873	0.459	10	132	12	130	40	45 duplicate
18348	141 Lanosta-8,24-dien-3-bet 85 [529; Methylcitric acid (1TMS)]	48	0.470	0.643	9.660	0.512	11	131	11	131	23	20 duplicate
19858	141 Lanosta-8,24-dien-3-bet 133 [855; Squalene]	61	0.463	0.609	13.504	0.494	12	130	13	129	53	25 duplicate
17675	141 Lanosta-8,24-dien-3-bet 74 [912; Tetradecanoic acid (1TMS)]	61	0.451	0.602	11.688	0.486	13	129	14	128	37	28 duplicate
19850	141 Lanosta-8,24-dien-3-bet 132 [895; Isomaltose methoxyamine (8TMS)]	39	0.425	0.475	10.262	0.447	14	128	20	122	27	55 duplicate
19325	141 Lanosta-8,24-dien-3-bet 107 [9-Z]-Octadecanoic acid	61	0.424	0.677	22.682	0.497	15	127	9	133	95	23 duplicate
15157	141 Lanosta-8,24-dien-3-bet 44 [910; 2-Ketogluconic acid methoxyamine (4TMS)]	47	0.397	0.560	14.833	0.453	16	126	16	126	63	48 duplicate
19715	141 Lanosta-8,24-dien-3-bet 122 [844; Erythritol (4TMS)]	49	0.396	0.568	8.828	0.486	17	125	15	127	13	29 duplicate
17471	141 Lanosta-8,24-dien-3-bet 71 [731; Erythrose (3TMS)]	61	0.372	0.381	20.250	0.407	18	124	26	116	88	95 duplicate
16846	141 Lanosta-8,24-dien-3-bet 60 Glycerol-3-phosphate	61	0.317	0.450	29.850	0.442	19	123	21	121	115	62 duplicate
19451	141 Lanosta-8,24-dien-3-bet 111 [583; Erythritol (4TMS)]	39	0.301	0.437	9.575	0.447	20	122	22	120	21	54 duplicate
19421	141 Lanosta-8,24-dien-3-bet 110 [715; Erythritol (4TMS)]	51	0.291	0.350	12.221	0.564	21	121	29	113	46	7 duplicate
18066	141 Lanosta-8,24-dien-3-bet 100 [857; Mannitol (6TMS)]	61	0.289	0.384	16.234	0.391	22	120	25	117	71	112 duplicate
19358	141 Lanosta-8,24-dien-3-bet 108 Octadecanoic acid	61	0.287	0.479	9.820	0.425	23	118	19	123	26	72 duplicate
17185	141 Lanosta-8,24-dien-3-bet 67 Citric acid	61	0.287	0.334	32.295	0.408	24	119	31	111	117	94 duplicate
18611	141 Lanosta-8,24-dien-3-bet 90 [910; 9-(Z)-Hexadecanoic acid (1TMS)]	61	0.268	0.506	14.108	0.402	25	117	18	124	57	99 duplicate
19876	141 Lanosta-8,24-dien-3-bet 136 [748; D-Sedheptulose-7-phosphate (7TMS)]	16	0.267	0.524	5.128	0.376	26	116	17	125	1	116 duplicate
19871	135 [902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]	61	0.258	0.431	20.338	0.457	27	115	23	119	89	46 duplicate

19145	141	Lanosta-8,24-dien-3-bet	102	[904; Galactose methoxyamine (5TMS)]	61	0,251	0,329	9,788	0,422	28	114	33	109	24	73 duplicate
19810	141	Lanosta-8,24-dien-3-bet	117	[724; Glycerol (3TMS)]	53	0,241	0,429	11,223	0,417	29	113	24	118	34	83 duplicate
18233	141	Lanosta-8,24-dien-3-bet	83	Sorbitol	56	0,230	0,141	28,983	0,363	30	112	59	83	111	130 duplicate
18480	141	Lanosta-8,24-dien-3-bet	112	[877; beta-D-Galactopyranoside-(1,2)-glycerol (6TMS)]	60	0,228	0,346	6,811	0,422	31	111	30	112	5	74 duplicate
12553	141	Lanosta-8,24-dien-3-bet	20	[819; 2-(3',4'-Bis(hydroxyphenyl)-2-oxoethylamine (4TMS)]	31	0,217	0,217	9,804	0,527	32	110	44	98	25	10 duplicate
18696	141	Lanosta-8,24-dien-3-bet	121	[657; Erythritol (4TMS)]	52	0,214	0,357	7,825	0,410	33	109	28	114	9	92 duplicate
18795	141	Lanosta-8,24-dien-3-bet	127	[777; Fructose-6-phosphate methoxyamine (6TMS)]	36	0,210	0,311	9,812	0,443	34	108	35	107	22	57 duplicate
18808	141	Lanosta-8,24-dien-3-bet	128	[824; D-Sedoheptulose-7-phosphate (7TMS)]	42	0,208	0,285	14,370	0,405	35	107	37	105	60	97 duplicate
18635	141	Lanosta-8,24-dien-3-bet	114	Fructose-6-phosphate	50	0,180	0,115	9,055	0,411	36	106	64	78	16	88 duplicate
12792	141	Lanosta-8,24-dien-3-bet	22	[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	50	0,177	0,331	7,176	0,427	37	105	32	110	7	70 duplicate
18961	141	Lanosta-8,24-dien-3-bet	115	Glucose-6-phosphate	59	0,175	-0,003	32,966	0,476	38	104	87	55	119	37 duplicate
15897	141	Lanosta-8,24-dien-3-bet	52	[NA]	43	0,169	0,376	11,845	0,455	39	103	27	115	39	47 duplicate
12310	141	Lanosta-8,24-dien-3-bet	18	[590; 1-Acetyl-2-thiohydantoin]	61	0,157	0,218	15,322	0,418	40	102	45	97	66	79 duplicate
14763	141	Lanosta-8,24-dien-3-bet	40	[680; 2,3-Dimethylsuccinic acid (2TMS)]	61	0,156	0,263	42,793	0,442	41	101	38	104	135	59 duplicate
13485	141	Lanosta-8,24-dien-3-bet	28	Malic acid	61	0,151	0,283	17,033	0,470	42	100	39	103	78	39 duplicate
18851	141	Lanosta-8,24-dien-3-bet	95	[770; 3,4,6-Tris(hydroxyphenyl)ethanolamine (5TMS)]	47	0,145	0,239	9,284	0,422	43	99	41	101	19	75 duplicate
10360	141	Lanosta-8,24-dien-3-bet	3	Ethanolamine	59	0,139	0,249	8,660	0,411	44	98	40	102	14	90 duplicate
14457	141	Lanosta-8,24-dien-3-bet	37	Phenylalanine	61	0,136	0,167	31,438	0,401	45	97	51	91	116	100 duplicate
19256	141	Lanosta-8,24-dien-3-bet	105	[705; 2-Ketogluconic acid (5TMS)]	45	0,135	0,317	16,748	0,462	46	96	34	108	73	43 duplicate
11557	141	Lanosta-8,24-dien-3-bet	12	Glycemic acid	60	0,130	0,197	7,039	0,432	48	94	47	95	6	68 duplicate
11812	141	Lanosta-8,24-dien-3-bet	14	Fumaric acid	61	0,127	0,228	7,800	0,412	49	93	43	99	10	87 duplicate
19291	141	Lanosta-8,24-dien-3-bet	106	[733; Threitol (4TMS)]	59	0,120	0,155	16,979	0,496	50	92	57	85	77	24 duplicate
13258	141	Lanosta-8,24-dien-3-bet	26	Citramalic acid	61	0,113	0,228	24,725	0,395	51	91	42	100	99	103 duplicate
12673	141	Lanosta-8,24-dien-3-bet	21	[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]	61	0,106	0,211	24,770	0,446	52	90	46	96	100	56 duplicate
18676	141	Lanosta-8,24-dien-3-bet	120	[945; Uridine (3TMS)]	51	0,106	0,009	19,746	0,417	53	89	84	58	85	81 duplicate
14863	141	Lanosta-8,24-dien-3-bet	41	[639; Proline (2TMS)]	61	0,102	0,161	21,853	0,453	54	88	55	87	92	60 duplicate
17933	141	Lanosta-8,24-dien-3-bet	78	Mannose	60	0,098	0,109	12,809	0,461	55	87	66	76	49	44 duplicate
19220	141	Lanosta-8,24-dien-3-bet	104	[795; Erythritol (4TMS)]	60	0,096	0,099	13,831	0,442	56	86	68	74	55	60 duplicate
19508	141	Lanosta-8,24-dien-3-bet	113	Galactose-6-phosphate	59	0,094	-0,094	11,998	0,381	57	85	108	34	42	115 duplicate
17870	141	Lanosta-8,24-dien-3-bet	77	[826; beta-[[[5-methyl-2-thienyl)methyl]amino- benzeneacetic acid methyl ester]	59	0,091	0,093	38,080	0,372	58	84	69	73	124	123 duplicate
17806	141	Lanosta-8,24-dien-3-bet	76	Fructose	61	0,090	-0,041	33,834	0,478	59	83	95	47	120	36 duplicate
18710	141	Lanosta-8,24-dien-3-bet	92	[680; Glycerol-2-phosphate (4TMS)]	51	0,089	-0,107	14,247	0,365	60	82	109	33	59	127 duplicate
18896	141	Lanosta-8,24-dien-3-bet	96	myo-Inositol	48	0,087	0,086	10,288	0,330	61	81	70	72	28	139 duplicate
18116	141	Lanosta-8,24-dien-3-bet	81	Tyrosine	61	0,082	0,183	42,564	0,482	62	80	50	92	134	32 duplicate
14353	141	Lanosta-8,24-dien-3-bet	36	[596; N-Acetylglutamic acid (2TMS)]	61	0,080	0,144	37,268	0,410	63	79	58	84	122	91 duplicate
14248	141	Lanosta-8,24-dien-3-bet	35	Pyroglutamic acid	61	0,074	-0,091	49,542	0,427	64	78	107	35	139	69 duplicate
12432	141	Lanosta-8,24-dien-3-bet	19	Alanine (BP) (3TMS)	61	0,067	0,048	20,076	0,474	65	77	77	65	87	38 duplicate
16158	141	Lanosta-8,24-dien-3-bet	55	[612; 4-Aminobutyric acid (2TBS)]	43	0,065	0,310	12,906	0,391	66	76	38	106	50	113 duplicate
14962	141	Lanosta-8,24-dien-3-bet	42	Glutamic acid	57	0,063	-0,017	36,031	0,406	67	75	89	53	123	96 duplicate
15718	141	Lanosta-8,24-dien-3-bet	50	[746; Ribonic acid-1,4-lactone (3TMS)]	58	0,055	0,189	8,992	0,428	68	74	48	94	15	68 duplicate
141	Lanosta-8,24-dien-3-bet														
16400	141	Lanosta-8,24-dien-3-bet	57	[757; 2-Desoxy-pentos-3-yose dimethoxyamine (2TMS)]	52	0,050	0,166	19,514	0,468	69	73	53	89	84	40 duplicate
16072	141	Lanosta-8,24-dien-3-bet	54	[NA]	52	0,039	0,065	10,862	0,339	70	72	73	69	32	137 duplicate
10902	141	Lanosta-8,24-dien-3-bet	7	Threonine	61	0,038	-0,001	38,907	0,453	71	71	86	56	129	49 duplicate
18290	141	Lanosta-8,24-dien-3-bet	84	Mannitol	59	0,036	-0,037	36,830	0,364	72	70	93	49	127	129 duplicate
17258	141	Lanosta-8,24-dien-3-bet	68	[570; Hypoxanthine (2TMS)]	20	0,032	0,159	9,293	0,420	73	69	56	86	18	77 duplicate
16805	141	Lanosta-8,24-dien-3-bet	62	[812; D-Xylofuranose (4TMS)]	61	0,030	-0,004	22,387	0,434	74	68	88	54	94	65 duplicate
17608	141	Lanosta-8,24-dien-3-bet	73	[708; Glucose methoxyamine (5TMS)]	55	0,028	0,128	12,334	0,412	75	67	63	79	47	85 duplicate
14560	141	Lanosta-8,24-dien-3-bet	38	[708; 2,3-Dimethylsuccinic acid (2TMS)]	61	0,021	0,167	15,054	0,440	76	66	52	90	64	63 duplicate

19841	141	Lanosta-8,24-dien-3-bet	131	[626; 5-Methylthioadenosine (3TMS)]	52	0,008	-0,167	9,124	0,502	77	65	116	26	17	22 duplicate
17401	141	Lanosta-8,24-dien-3-bet	70	[693; 2-Furan-2-hydroxyacetic acid (2TMS)]	55	0,007	-0,112	25,959	0,358	78	64	110	32	105	134 duplicate
19733	141	Lanosta-8,24-dien-3-bet	123	[945; Galactofuranose-6-phosphate (7TMS)]	61	-0,001	-0,083	19,230	0,417	79	63	103	39	82	82 duplicate
11428	141	Lanosta-8,24-dien-3-bet	11	Succinic acid	61	-0,012	0,015	15,551	0,396	80	62	83	59	67	102 duplicate
15808	141	Lanosta-8,24-dien-3-bet	51	[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid (2TMS)]	43	-0,014	-0,090	11,375	0,357	81	61	105	37	35	135 duplicate
15985	141	Lanosta-8,24-dien-3-bet	53	Glycerol-2-phosphate	61	-0,015	-0,056	7,563	0,419	82	60	97	45	8	78 duplicate
19766	141	Lanosta-8,24-dien-3-bet	125	[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]	61	-0,016	-0,239	40,440	0,370	83	59	124	18	131	126 duplicate
17540	141	Lanosta-8,24-dien-3-bet	72	[919; D-Xylopyranose (4TMS)]	60	-0,018	-0,091	12,063	0,334	84	58	106	36	43	138 duplicate
16565	141	Lanosta-8,24-dien-3-bet	59	Ornithine; Arginine	61	-0,019	-0,116	49,621	0,365	85	57	112	30	140	128 duplicate
19820	141	Lanosta-8,24-dien-3-bet	129	Glc	56	-0,019	0,140	15,926	0,519	86	56	60	82	69	12 duplicate
18401	141	Lanosta-8,24-dien-3-bet	86	[793; D-Galactono-1,4-lactone (4TMS)]	59	-0,020	-0,047	28,693	0,519	87	55	96	46	110	13 duplicate
19633	141	Lanosta-8,24-dien-3-bet	118	[928; Glucopyranose-6-phosphate (6TMS)]	55	-0,021	-0,159	12,164	0,425	88	54	115	27	45	71 duplicate
17330	141	Lanosta-8,24-dien-3-bet	69	Arginine	58	-0,024	-0,118	29,782	0,464	89	53	114	28	114	41 duplicate
18831	141	Lanosta-8,24-dien-3-bet	130	Trehalose	60	-0,024	0,003	38,561	0,362	90	52	85	57	125	133 duplicate
16726	141	Lanosta-8,24-dien-3-bet	61	[NA]	61	-0,033	0,060	13,003	0,326	91	51	75	67	51	140 duplicate
18758	141	Lanosta-8,24-dien-3-bet	93	[607; Putrescine (4TMS)]	58	-0,038	-0,058	10,352	0,412	92	50	98	44	29	86 duplicate
11298	141	Lanosta-8,24-dien-3-bet	10	Glycine	61	-0,040	-0,079	27,668	0,483	93	49	102	40	108	31 duplicate
14662	141	Lanosta-8,24-dien-3-bet	39	[829; 1-Phenylethanol (1TMS)]	60	-0,047	0,165	22,915	0,449	94	48	54	88	96	52 duplicate
17036	141	Lanosta-8,24-dien-3-bet	55	[646; 3-Deoxyglucitol (5TMS)]	60	-0,049	0,064	16,298	0,491	95	47	74	68	72	26 duplicate
18508	141	Lanosta-8,24-dien-3-bet	88	Gluconic acid	61	-0,055	0,017	19,493	0,513	96	45	81	61	83	19 duplicate
15348	141	Lanosta-8,24-dien-3-bet	46	Arabinose	61	-0,055	-0,027	24,346	0,488	97	46	91	51	98	27 duplicate
11685	141	Lanosta-8,24-dien-3-bet	13	Uracil	61	-0,061	0,026	32,585	0,513	99	42	80	62	118	18 duplicate
15535	141	Lanosta-8,24-dien-3-bet	134	Isomaltose	61	-0,061	-0,039	17,366	0,485	100	43	94	48	79	30 duplicate
18940	141	Lanosta-8,24-dien-3-bet	97	[756; beta-D-Methylglucopyranoside (4TMS)]	49	-0,061	-0,115	27,372	0,377	101	41	111	31	107	118 duplicate
13597	141	Lanosta-8,24-dien-3-bet	29	Erythritol	61	-0,069	0,073	11,763	0,463	102	40	72	70	38	42 duplicate
16316	141	Lanosta-8,24-dien-3-bet	56	[829; Orolic acid (3TMS)]	50	-0,082	0,016	40,925	0,371	104	38	82	60	132	125 duplicate
10497	141	Lanosta-8,24-dien-3-bet	4	Phosphoric acid	49	-0,088	0,188	14,391	0,431	105	37	49	93	61	67 duplicate
16883	141	Lanosta-8,24-dien-3-bet	63	Glutamine	60	-0,089	-0,066	19,942	0,376	106	36	101	41	86	120 duplicate
13708	141	Lanosta-8,24-dien-3-bet	30	[815; Ethyl-3-(2H)-thiophenone]	61	-0,091	-0,196	38,861	0,404	107	35	122	20	128	98 duplicate
17741	141	Lanosta-8,24-dien-3-bet	75	Lysine	61	-0,103	-0,085	48,421	0,381	108	34	104	38	138	116 duplicate
18175	141	Lanosta-8,24-dien-3-bet	82	Lysine	39	-0,107	-0,193	21,463	0,509	109	33	121	21	91	21 duplicate
15627	141	Lanosta-8,24-dien-3-bet	49	[877; Pyrophosphoric acid (4TMS)]	61	-0,108	-0,180	14,538	0,363	110	32	120	22	62	131 duplicate
13927	141	Lanosta-8,24-dien-3-bet	32	[729; N,N-Dimethyllysine methyl ester]	60	-0,110	-0,116	15,227	0,451	111	31	113	29	65	51 duplicate
12063	141	Lanosta-8,24-dien-3-bet	16	[644; 2-Methyl-1,3-butanediol (2TMS)]	61	-0,111	0,048	25,929	0,519	112	30	76	66	104	15 duplicate
13027	141	Lanosta-8,24-dien-3-bet	24	[725; 2-Ketotetrandic acid (2TMS)]	61	-0,114	0,040	40,102	0,522	113	29	79	63	130	11 duplicate
18455	141	Lanosta-8,24-dien-3-bet	87	[945; beta-D-Glucopyranose (5TMS)]	59	-0,115	-0,186	42,946	0,363	114	28	119	23	138	132 duplicate
14035	141	Lanosta-8,24-dien-3-bet	33	Methionine	61	-0,117	-0,203	17,604	0,411	115	27	123	19	80	88 duplicate
16483	141	Lanosta-8,24-dien-3-bet	58	[636; 4R-Acetalmito-2,3-(2Z)-epoxy-4(E)-hydroxycyclohexane (1TMS)]	61	-0,122	-0,173	24,836	0,418	116	26	118	24	101	80 duplicate
11167	141	Lanosta-8,24-dien-3-bet	9	Proline	61	-0,129	-0,020	35,861	0,394	117	25	90	52	121	106 duplicate
19025	141	Lanosta-8,24-dien-3-bet	99	[662; Ribose-5-phosphate methoxyamine (BP) (5TMS)]	38	-0,132	0,111	8,595	0,480	118	24	65	77	12	35 duplicate
11035	141	Lanosta-8,24-dien-3-bet	8	Isoleucine	53	-0,139	0,135	25,471	0,360	119	23	61	81	102	117 duplicate
17111	141	Lanosta-8,24-dien-3-bet	66	Glycine acid-3-phosphate	61	-0,145	-0,066	10,871	0,443	120	21	100	42	33	58 duplicate
13818	141	Lanosta-8,24-dien-3-bet	31	[622; Parabanic acid (2TMS)]	61	-0,145	-0,170	9,396	0,393	121	22	117	25	20	108 duplicate
10633	141	Lanosta-8,24-dien-3-bet	5	Leucine	45	-0,145	-0,373	12,525	0,400	122	20	138	4	48	101 duplicate
14142	141	Lanosta-8,24-dien-3-bet	34	Aspartic acid	61	-0,149	-0,262	41,698	0,392	123	19	127	15	133	110 duplicate
12187	141	Lanosta-8,24-dien-3-bet	17	[700; 2-methyl-1,2-propanediol (2TMS)]	61	-0,168	-0,064	25,899	0,421	124	18	99	43	103	76 duplicate
10768	141	Lanosta-8,24-dien-3-bet	6	Glycerol	61	-0,181	-0,322	50,195	0,392	125	17	131	11	141	109 duplicate

18580	141	Lanosta-8,24-dien-3-bet	89	[775; Dopamine (4TMS)]	34	-0,184	0,104	13,977	0,415	128	16	67	75	56	84 duplicate
18056	141	Lanosta-8,24-dien-3-bet	80	[772; D-Glucose (5TMS)]	59	-0,184	-0,278	38,701	0,321	127	15	130	12	128	141 duplicate
10222	141	Lanosta-8,24-dien-3-bet	2	Serine	59	-0,189	0,042	26,345	0,409	128	14	78	64	106	93 duplicate
15253	141	Lanosta-8,24-dien-3-bet	45	Homocysteine	58	-0,204	-0,328	12,093	0,343	129	13	132	10	44	136 duplicate
19106	141	Lanosta-8,24-dien-3-bet	101	[832; Dopamine (4TMS)]	61	-0,215	-0,243	18,913	0,394	130	12	125	17	76	105 duplicate
18661	141	Lanosta-8,24-dien-3-bet	91	[766; beta-D-Methylglucopyranoside (4TMS)]	61	-0,216	-0,269	22,058	0,387	131	11	129	13	93	114 duplicate
17895	141	Lanosta-8,24-dien-3-bet	79	Glucose	61	-0,220	-0,336	43,763	0,392	132	10	133	9	137	111 duplicate
16960	141	Lanosta-8,24-dien-3-bet	64	[789; Tyramine (3TMS)]	60	-0,235	-0,337	11,887	0,434	133	9	134	8	41	84 duplicate
15442	141	Lanosta-8,24-dien-3-bet	47	[NA]	61	-0,259	-0,350	16,820	0,375	134	8	137	5	74	121 duplicate
18983	141	Lanosta-8,24-dien-3-bet	98	[697; Ribose-5-phosphate methoxyamine (5TMS)]	45	-0,261	-0,267	11,502	0,395	135	7	128	14	36	104 duplicate
10083	141	Lanosta-8,24-dien-3-bet	1	[938; Sulfuric acid (2TMS)]	33	-0,261	-0,257	10,517	0,442	136	6	126	16	30	61 duplicate
12910	141	Lanosta-8,24-dien-3-bet	23	Homoserine	61	-0,278	-0,346	18,076	0,447	137	5	136	6	81	53 duplicate
15060	141	Lanosta-8,24-dien-3-bet	43	[548; Leucine (2TBS)]	58	-0,286	-0,459	16,014	0,371	138	4	139	3	70	124 duplicate
11938	141	Lanosta-8,24-dien-3-bet	15	Alanine	61	-0,302	-0,487	27,700	0,480	139	3	140	2	109	34 duplicate
13372	141	Lanosta-8,24-dien-3-bet	27	[815; (E)-4-Methyl-5-hydroxy-3-pentien-2-one (1TMS)]	51	-0,307	-0,343	15,835	0,393	140	2	135	7	68	107 duplicate
13143	141	Lanosta-8,24-dien-3-bet	25	[709; 2,5-Diaminovalerolactam (2TMS)]	45	-0,410	-0,554	16,902	0,516	141	1	141	1	75	16 duplicate

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